APPENDIX 1: AE3 PROGRAM

```
1 FTVSCLR PROGRAM=%H! DATA=.PDP:INPUT NAG
2 C
3 C PROGRAM FOR THE CALCULATION OF THE AE3 TEMPERATURE
4 C FOR LOW-ALLOY STEELS
5 C COPYRIGHT A.A.B.SUGDEN 1985.
6 C ELEMENTS MUST BE INSERTED IN THE DATASET IN THE ORDER:
7 C Mn Si Ni Cr Mo Cu V Nb W Co
8 C
9 IMPLICIT DOUBLE PRECISION (T)
10 DOUBLE PRECISION A(10),AC,AI(10),B(10,5),C,C6,CAF,CF,CLIQ,D(10,6)
11 DOUBLE PRECISION DAT(10),DELTAT,DTALPH,DTGAM,E(10,4),FEAF,G,GC,GI
12 DOUBLE PRECISION H,H1,P,Q,R,WTPC,X(10),XX(10),Z,Z6,Z61
13 DOUBLE PRECISION HK(13),HC(13)
14 COMMON /INTER/B
15 COMMON /DELTA2/E
16 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,H1,H
17 INTEGER ANS,COUNT,COUNTA,DUMMY,FLAG1,FLAG2,S43,S54,S91
18 COUNTA = 2
19 K = 2
20 MM = 2
21 NCAP7 = 13
22 IFAIL = 0
23 R = 1.9858D0
24 C cal/mol/K
25 DATA C, SUM, DELTAT/0.0D0, 0.0D0, 0.0D0/
26 DATA TEMP, TT, Z/0.0D0, 0.0D0, 0.0D0/
27 C
28 C SPLINE COEFFICIENTS FOR DELTAoHo
29 C INTERPOLATES DATA FROM KAUFMAN ET AL. (RANGE 0-1183K)
30 C
31 DATA HK(1),HK(2),HK(3),HK(4)/0.0D0,0.0D0,0.0D0,0.0D0/,
32 * HK(5),HK(6),HK(7),HK(8),HK(9)/1.5D2,3.0D2,7.2D2,9.6D2,1.08D3/,
33 * HK(10),HK(11),HK(12),HK(13)/1.183D3,1.183D3,1.183D3,1.183D3/,
34 * HC(1),HC(2),HC(3),HC(4)/1.303D3,1.272D3,1.368D3,1.703D3/,
35 * HC(5),HC(6),HC(7),HC(8)/1.552D3,1.281D3,3.359D2,2.344D2/,
36 * HC(9),HC(10),HC(11),HC(12)/2.134D2,0.0D0,0.0D0,0.0D0/,
37 * HC(13)/0.0D0/
38 ************************************************
```

```
39 WRITE(6,101)
40 WRITE(6,51)
41 WRITE(6,301)
42 WRITE(6,51)
43 READ(5,*) (DAT(I),I=1,10)
44 IF (ADD(DAT).EQ.0.0D0) THEN
45 WRITE(6,159)
46 ELSE
47 WRITE(6,160)
48 IF (DAT(1).NE.0.0D0) WRITE(6,161)DAT(1)
49 IF (DAT(2).NE.0.0D0) WRITE(6,162)DAT(2)
50 IF (DAT(3).NE.0.0D0) WRITE(6,163)DAT(3)
51 IF (DAT(4).NE.0.0D0) WRITE(6,164)DAT(4)
52 IF (DAT(5).NE.0.0D0) WRITE(6,165)DAT(5)
53 IF (DAT(6).NE.0.0D0) WRITE(6,166)DAT(6)
54 IF (DAT(7).NE.0.0D0) WRITE(6,167)DAT(7)
55 IF (DAT(8).NE.0.0D0) WRITE(6,168)DAT(8)
56 IF (DAT(9).NE.0.0D0) WRITE(6,169)DAT(9)
57 IF (DAT(10).NE.0.0D0) WRITE(6,170)DAT(10)
58 ENDIF
59 101 FORMAT(1X)
60 301 FORMAT(' A e 3 P R O G R A
61 1 M')
62 159 FORMAT(' Pure iron')
63 160 FORMAT(' The steel contains:')
64 161 FORMAT(F5.2,' wt% manganese')
65 162 FORMAT(F5.2,' wt% silicon')
66 163 FORMAT(F5.2,' wt% nickel')
67 164 FORMAT(F5.2,' wt% chromium')
68 165 FORMAT(F5.2,' wt% molybdenum')
69 166 FORMAT(F5.2,' wt% copper')
70 167 FORMAT(F5.2,' wt% vanadium')
71 168 FORMAT(F5.2,' wt% niobium')
72 169 FORMAT(F5.2,' wt% tungsten')
73 170 FORMAT(F5.2,' wt% cobalt')
74 ******************************************************
75 DO 1 I = 1,10
76 1 XX(I) = DAT(I)
77 C wt%
```

```
78 DUMMY = 0
79 2 C6 = 0.0D0
80 NUM = 0
81 COUNT = 0
82 FLAG2 = 1
83 DTGAM = 0.0D0
84 Z61 = 1.0D2
85
86 WRITE(6,52)
87 WRITE(6,57)
88 WRITE(6,55)
89 WRITE(6,57)
90 3 CONTINUE
91 DO 17 N = 1,51
92 IF (COUNT.EQ.-1 .OR. COUNT.EQ.12) GOTO 17
93 IF (K.EQ.5 .AND. NUM.EQ.3) GOTO 17
94 C = (N-1)*0.01D0
95 4 CONTINUE
96 5 WTPC = C + ADD(XX)
97 IF (WTPC.GT.5.0) THEN
98 WRITE(6,52)
99 WRITE(6,53)
100 88 WRITE(6,54)
101 GOTO 88
102 ENDIF
103 C
104 C CALCULATION OF MOLE FRACTIONS
105 C
106 FEAF = (1.0D2-WTPC)/5.58D1
107 CAF = C/1.2D1
108 DO 6 M = 1,10
109 6 X(M) = XX(M)/B(M,1)
110 TAF = FEAF + CAF + ADD(X)
111 CF = CAF/TAF
112 DO 7 M = 1,10
113 7 X(M) = X(M)/TAF
114 CALL TZERO (CF,TO)
115 T = TO
116 H1 = -1.5325D4
```

```
117 11 CONTINUE
118 CALL GALGA(G,GC,T)
119 G = -G
120 IF (T.GT.1.183D3) THEN
121 C
122 C VALID UP TO 1360K
123 C
124 H = 2.549D3 - 2.746D0*T + 6.503D-4*T*T
125 G = 2.476D3-5.03D0*T+3.363D-3*T*T-7.44D-7*T*T*T
126 ELSE
127 CALL E02BBF(NCAP7,HK,HC,T,H,IFAIL)
128 ENDIF
129 AC = DEXP(GC/(R*TO)+(8.91D3/T)*CF)
130
131 SUM = 0.0D0
132 DELTAT = 0.0D0
133 DO 14 M = 1,10
134 IF (X(M).EQ.0) THEN
135 A(M)=0.0D0
136 AI(M)=1.0D0
137 GOTO 14
138 ENDIF
139
140 P = B(M,4) + B(M,5)/T
141 Q = 0.0D0
142 IF (M.EQ.1) THEN
143 C
144 C DATA FROM GILMOUR ET AL., MET. TRANS., 1972
145 C
146 GI = 6.118*T - 7808.0
147 ELSE
148 GI = E(M,1)+(E(M,2)+E(M,3)*T+E(M,4)*DLOG(T))*T
149 ENDIF
150
151 C
152 C CALCULATION FOR SOLUTE PARTITION COEFFICIENTS
153 C
154 AI(M) = DEXP(GI/(R*TO)+P*CF)
155
```

```
156 CALL EQN(A(M),K,C,CLIQ)
157 SUM = SUM + X(M)*A(M)
158 14 CONTINUE
159 DELTAT = SUM*R*TO*TO
160 T = TO+DELTAT
161 Z = TT - T
162 Z = DABS(Z)
163 IF (Z.LT.0.5D0) GOTO 15
164 TT = T
165 IF (K.EQ.2) GOTO 11
166 15 CONTINUE
167
168 IF (COUNT.EQ.-1) THEN
169 IF (DUMMY.NE.0) TEMP = T
170 GOTO 17
171 ENDIF
172 IF (K.EQ.3 .AND. S93.NE.3) THEN
173 WRITE(6,51)
174 ELSE
175 IF (S91.EQ.3 .AND. N.EQ.1) GOTO 17
176 IF (NUM.EQ.1) THEN
177 IF (T.LT.TEMP) THEN
178 COUNT = -1
179 GOTO 17
180 ELSE
181 WRITE(6,51)
182 ENDIF
183 ELSE
184 WRITE(6,63)C,T-273,AC
185 DO 16 I = 1,10
186 IF (AI(I).EQ.1.0D0) GOTO 16
187 IF (I.LT.9) THEN
188 WRITE(6,65)I+1,AI(I)
189 ELSE
190 WRITE(6,66)I+1,AI(I)
191 ENDIF
192 16 CONTINUE
193 ENDIF
194 ENDIF
```

```
195 17 CONTINUE
196 STOP
197
198 51 FORMAT(1X,62(1H-))
199 52 FORMAT(1X)
200 53 FORMAT(' The sum of the alloy components should not exceed 5wt%.')
201 54 FORMAT(1X,80(1H ))
202 55 FORMAT(' WT%C T/degreesC Partition coefficients')
203 57 FORMAT(' +————————————+————————————
204 1—+')
205 63 FORMAT(' ',F5.2,' ',F6.1,' A(c) :',F6.3)
206 65 FORMAT(' A(',I1,') :',F6.3)
207 66 FORMAT(' A(',I2,'):',F6.3)
208 END
209
210 C
211 C DATA FOR ALLOYING ELEMENT INTERACTION PARAMETERS
212 C
213 BLOCK DATA ETA
214 COMMON /INTER/B
215 DOUBLE PRECISION B(10,5)
216 DATA((B(M,J),J=1,5),M=1,10)/
217 C5.49D1,0.0D0,-5.06D3,0.0D0,-5.07D3,
218 C2.81D1,-4.28D-1,1.874D4,4.84D0,-7.37D3,
219 C5.87D1,0.0D0,5.34D3,-2.2D0,7.6D3,
220 C5.20D1,0.0D0,-9.5D3,2.44D1,-3.84D4,
221 C9.59D1,0.0D0,-7.49D3,3.855D0,-1.787D4,
222 C6.35D1,0.0D0,7.586D3,0.0D0,4.2D3,
223 C5.09D1,0.0D0,-3.01D4,0.0D0,-2.466D4,
224 C9.29D1,0.0D0,-4.6615D4,0.0D0,-2.877D4,
225 C1.838D2,0.0D0,-1.223D4,2.34D1,-3.6214D4,
226 C5.89D1,0.0D0,3.55D3,0.0D0,2.8D3/
227 END
228
229 C
230 C DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))
231 C [FERRITE-AUSTENITE TRANSORMATION]
232 C
233 BLOCK DATA DGI2
```

```
234 COMMON /DELTA2/E
235 DOUBLE PRECISION E(10,4)
236 DATA((E(M,J),J=1,4),M=1,10)/
237 C-2.665D4,4.269D1,-1.7D-2,0.0D0,      Mn
238 C-5.964D3,3.8799D1,0.0D0,-4.7244D0,  Si
239 C-4.545D3,3.233D0,0.0D0,0.0D0,       Ni
240 C-3.67D2,-4.656D0,0.0D0,6.568D-1,    Cr
241 C5.65D2,1.5D-1,0.0D0,0.0D0,          Mo
242 C-2.55D4,4.1183D1,-1.7D-1,0.0D0,     Cu
243 C-8.357D3,1.38D1,-5.1D-3,0.0D0,      V
244 C
245 C NIOBIUM RECALCULATED
246 C REF: A.A.B.SUGDEN, C.P.G.S DISSERTATION, 1986
247 C
248 C5.139D3,-2.892D0,0.0D0,0.0D0,  Nb   Calc wrong
249 C2.5D3,1.5D-1,0.0D0,0.0D0,      W
250 C0.0D0,0.0D0,0.0D0,0.0D0/       Co
251 END
252
253 DOUBLE PRECISION FUNCTION ADD(Y)
254 DOUBLE PRECISION Y(10)
255 ADD = 0.0D0
256 DO 4 I = 1,10
257 4 ADD = ADD + Y(I)
258 RETURN
259 END
260
261 ******************************************************
262 C
263 C THIS SECTION CONTAINS 2 SUBROUTINES TO FIND
264 C To AND DELTAGo RESPECTIVELY
265 C
266 SUBROUTINE TZERO (X1,T1)
267 C
268 C DATA PROVIDED BY BHADESHIA
269 C RANGE 200-900 CENTIGRADE
270 C
271 DOUBLE PRECISION X1,T1
272 IF (X1.GE.6.88D-2) GOTO 1
```

```
273 IF (X1.LT.1.0D-3) THEN
274 T1 = 9.115D2 - 2.12D4*X1 + 3.45D6*X1*X1
275 ELSE
276 IF (X1.LT.3.135D-2) THEN
277 T1 = 9.056D2-1.068D4*X1+2.811D5*X1*X1-3.913D6*(X1**3)
278 ELSE
279 IF (X1.LT.4.84D-2) THEN
280 T1 = 8.558D2 - 4.694D3*X1 + 2.156D4*X1*X1
281 ELSE
282 T1 = 7.475D2 - 1.449D3*X1 - 7.163D3*X1*X1
283 ENDIF
284 ENDIF
285 ENDIF
286 GOTO 2
287 1 CONTINUE
288 IF (X1.LT.9.33D-2) THEN
289 T1 = 6.152D2 + 1.779D3*X1 - 2.677D4*X1*X1
290 ELSE
291 IF (X1.LT.1.526D-1) THEN
292 T1 = 5.168D2 + 5.017D3*X1 - 6.693D4*X1*X1
293 T1 = T1 + 1.823D5*(X1**3)
294 ELSE
295 T1 = 6.922D2 - 1.087D3*X1 - 6.696D3*X1*X1
296 ENDIF
297 ENDIF
298 2 CONTINUE
299 T1 = T1 + 273
300 RETURN
301 END
302
303 SUBROUTINE GALGA (G2,GC2,T2)
304 C
305 C DATA DUE TO KAUFMAN, CLOUGHERTY, AND WEISS
306 C (RANGE 0-1183K)
307 C
308 DOUBLE PRECISION G2,GC2,T2
309 IF (T2.LT.7.0D2) THEN
310 IF (T2.LT.3.0D2) THEN
311 G2 = 1.38D0*T2 - 1.499D3
```

```
312 ELSE
313 G2 = 1.65786D0*T2 - 1.581D3
314 ENDIF
315 ELSE
316 IF (T2.LT.9.4D2) THEN
317 G2 = 1.30089D0*T2 - 1.331D3
318 ELSE
319 G2 = - 8.89909D0 + 2.6557D-1*(T2-1.14D3)
320 G2 = G2 - 1.04923D-3*(T2-1.14D3)*(T2-1.14D3)
321 G2 = G2 + 2.70013D-6*((T2-1.14D3)**3)
322 G2 = G2 - 3.58434D-9*((T2-1.14D3)**4)
323 C
324 C CORRECTED DATA PROVIDED BY BHADESHIA AND YANG
325 C
326 ENDIF
327 ENDIF
328 GC2 = 7.686D0*T2 - 1.5325D4
329 RETURN
330 END
331 ******************************************************
332
333 SUBROUTINE EQN (F16,NO,CC,CQIL)
334 IMPLICIT DOUBLE PRECISION (F)
335 DOUBLE PRECISION G,R,TO,T,P,CF,Q,GC,GI,H1,H
336 DOUBLE PRECISION CC,CQIL,EG11,EL11
337 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,H1,H
338 C
339 C SET CARBON-CARBON INTERACTION PARAMETERS
340 C
341 EG11 = 0.0D0
342 EL11 = 8.91D3/T
343 C
344 C MAIN EQUATION
345 C
346 F1 = GI/(R*TO) + P*CF
347 F2 = GC/(R*TO)
348 F3 = 1 + Q*CF*DEXP(F2)
349 F4 = GC/(R*TO) + (EL11)*CF
350 F5 = 1 + EG11*CF*DEXP(F2)
```

```
351 F6 = DEXP(F1)/F3
352 F7 = DEXP(F4)/F5
353 F8 = 1+CF*(1-CF)*(P-Q*F6*F7)
354 F9 = G/(R*TO*TO)
355 F10 = CF*CF/2*((EL11)-(EG11*F7*F7))
356 F11 = DEXP(F4)*CF*H1/F5
357 F12 = (1-CF)*H
358 F13 = F9 - F10
359 F14 = F11+F12*DEXP(F13)
360 F15 = F8*DEXP(F13)
361 F16 = (F6-F15)/F14
362 RETURN
363 END
364 !
```

APPENDIX 2: DETERMINATION OF ΔT

The chemical potentials in the two phases are equal. Therefore, *e.g.*, for the austenite liquidus.

$$X_\circ^\gamma \gamma_\circ^\gamma = X_\circ^L \gamma_\circ^L \exp\left(\frac{\Delta^\circ G_\circ^{\gamma \to L}}{RT}\right)$$

Therefore

$$\frac{\Delta^\circ G_\circ^{\gamma \to L}}{RT} = \ln\left|\frac{X_\circ^\gamma}{X_\circ^L}\right| + \ln|\gamma_\circ^\gamma| - \ln|\gamma_\circ^L| \tag{1}$$

Similarly, for the i^{th} component

$$X_i^\gamma \gamma_i^\gamma = X_i^L \gamma_i^L \exp\left(\frac{\Delta^\circ G_i^{\gamma \to L}}{RT}\right)$$

Therefore

$$\frac{\Delta^\circ G_i^{\gamma \to L}}{RT} = \ln\left|\frac{X_i^\gamma}{X_i^L}\right| + \ln|\gamma_i^\gamma| - \ln|\gamma_i^L|$$

The Wagner (Taylor) activity formulae for a ternary system, with the standard state defined at infinite dilution, may be written

$$\ln \gamma_\circ = -\frac{1}{2} \sum_{i,\ k=1}^{n} \epsilon_{ik} X_i X_k$$

and $$\ln \gamma_i = \sum_{2}^{n} \epsilon_{ik} X_k$$

For Fe ($n = 0$)

$$X_\circ^\gamma = 1 - X_1^\gamma - \sum_{2}^{n} X_i^\gamma$$

and $$X_\circ^L = 1 - X_1^L - \sum_{2}^{n} X_i^L$$

Therefore, from Eqn. (1)

$$\frac{\Delta^\circ G_\circ^{\gamma \to L}}{RT} = \ln \left| \frac{1 - X_1^\gamma - \sum_{2}^{n} X_i^\gamma}{1 - X_1^L - \sum_{2}^{n} X_i^L} \right| - \frac{\epsilon_{11}^\gamma}{2} (X_1^\gamma)^2$$

$$- X_1^\gamma \sum_{2}^{n} \epsilon_{1i}^\gamma X_i^\gamma + \frac{\epsilon_{11}^L}{2} (X_1^L)^2 + X_1^L \sum_{2}^{n} \epsilon_{1i}^L X_i^L \qquad (2)$$

Similarly, for C ($n = 1$)

$$\frac{\Delta^\circ G_1^{\gamma \to L}}{RT} = \ln \left| \frac{X_1^\gamma}{X_1^L} \right| + \epsilon_{11}^\gamma X_1^\gamma - \epsilon_{11}^L X_1^L \qquad (3)$$

and for component i

$$\frac{\Delta^\circ G_i^{\gamma \to L}}{RT} = \ln \left| \frac{X_i^\gamma}{X_i^L} \right| + \epsilon_{1i}^\gamma X_i^\gamma - \epsilon_{1i}^L X_i^L$$

Rearranging Eqn. (3) gives

$$X_1^\gamma \exp(\epsilon_{11}^\gamma X_1^\gamma) = X_1^L \exp \left[\frac{\Delta^\circ G_1^{\gamma \to L}}{RT} + \epsilon_{11}^L X_1^L \right] \tag{4}$$

Similarly, for component i

$$X_i^\gamma \exp(\epsilon_{1i}^\gamma X_i^\gamma) = X_i^L \exp \left[\frac{\Delta^\circ G_i^{\gamma \to L}}{RT} + \epsilon_{1i}^L X_i^L \right] \tag{5}$$

Now

$$\exp \left[\frac{\Delta^\circ G_{(T)}}{RT} \right] = \exp \left[-\frac{\Delta^\circ S}{R} \right] \exp \left[\frac{\Delta^\circ H}{RT} \right]$$

Let $T = T_\circ + \Delta T$. Then

$$\exp \left[\frac{\Delta^\circ G_{(T)}}{RT} \right] = \exp \left[-\frac{\Delta^\circ S}{R} \right] \exp \left[\frac{\Delta^\circ H \circ}{T_\circ} \right] \exp \left[-\frac{\Delta^\circ H_\circ}{T_\circ} \right] \exp \left[\frac{\Delta^\circ H}{R(T_\circ + \Delta T)} \right]$$

$$= \exp \left[\frac{\Delta^\circ G_\circ}{RT_\circ} \right] \exp \left[\frac{\Delta^\circ H T_\circ - \Delta^\circ H(T_\circ + \Delta T)}{RT_\circ(T_\circ + \Delta T)} \right]$$

Likewise

$$\exp\left[\frac{\Delta^\circ G_1}{RT}\right] = \exp\left[\frac{\Delta^\circ G_1}{RT_\circ}\right] \exp\left[\frac{-\Delta^\circ H \Delta T}{RT_\circ(T_\circ + \Delta T)}\right]$$

At $T = T_\circ$

$$\exp\left[\frac{\Delta^\circ G_i}{RT}\right] = \exp\left[\frac{\Delta^\circ G_i}{RT_\circ}\right]$$

Therefore from Eqn. (4)

$$\begin{aligned} X_1^\gamma \exp(\epsilon_{11}^\gamma X_1^\gamma) &= X_1^L \exp\left[\frac{\Delta^\circ G_1^{\gamma \to L}}{RT}\right] \exp(\epsilon_{11}^L X_1^L) \\ &= X_1^L \exp\left[\frac{\Delta^\circ G_1}{RT_\circ}\right] \exp\left[\frac{-\Delta^\circ H_1 \Delta T}{RT_\circ(T_\circ + \Delta T)}\right] \exp(\epsilon_{11}^L X_1^L) \\ &= X_1^L \exp\left[\frac{\Delta^\circ G_1}{RT_\circ} - \frac{\Delta^\circ H_1 \Delta T}{RT_\circ(T_\circ + \Delta T)} + (\epsilon_{11}^L X_1^L)\right] \end{aligned} \tag{6}$$

and Eqn. (5) may be written

$$X_i^\gamma \exp(\epsilon_{1i}^\gamma X_i^\gamma) = X_i^L \exp\left[\frac{\Delta^\circ G_1^{\gamma \to L}}{RT} + \epsilon_{1i}^L X_i^L\right] \tag{7}$$

Substituting for $\left[\frac{\Delta^\circ G_o}{RT}\right]$ in Eqn. (2) and rearranging gives the final equation

$$\frac{\Delta^\circ G_o}{RT_\circ} - \frac{\Delta^\circ H_\circ \Delta T}{RT_\circ(T + \Delta T)}$$

$$- \ln|1 - X_1^\gamma - \sum_{i=2}^{n} X_i^\gamma| + \ln|1 - X_1^L - \sum_{i=2}^{n} X_i^L|$$

$$+ \frac{\epsilon_{11}^\gamma}{2}(X_1^\gamma)^2 - X_1^\gamma \sum_{i=2}^{n} \epsilon_{1i}^\gamma X_i^\gamma + \frac{\epsilon_{11}^L}{2}(X_1^L)^2 - X_1^L \sum_{i=2}^{n} \epsilon_{1i}^L X_i^L = 0 \qquad (8)$$

X_1^γ and X_i^γ are found from (6) and (7) respectively.

APPENDIX 3: PERITECTIC PROGRAM

```
1 FTVSCLR %H% DATA=.DATA NAG OUTPUT=.OUT
2 C
3 C PROGRAM TO CACULATE THE PERITECTIC REGION OF THE
4 C IRON-CARON PHASE DIAGRAM FOR ANY GIVEN LOW ALLOY STEEL.
5 C COPYRIGHT A. A. B. SUGDEN 1988.
6 C ELEMENTS MUST BE PLACED IN THE DATASET IN THE ORDER:
7 C Mn Si Ni Cr Mo Cu V Nb W Co
8 C
9 IMPLICIT DOUBLE PRECISION (T)
10 DOUBLE PRECISION A(10),AC,AI(10),B(10,5),C,C6,CAF,CF,CLIQ,D(10,6)
11 DOUBLE PRECISION DAT(10),DELTAT,DTALPH,DTGAM,E(10,4),FEAF,G,GC,GI
12 DOUBLE PRECISION H,HC,P,Q,R,WTPC,X(10),XX(10),Z,Z6,Z61
13 COMMON /INTER/B
14 COMMON /DELTA1/D
15 COMMON /DELTA2/E
16 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,HC,H
17 INTEGER ANS,COUNT,COUNTA,DUMMY,FLAG1,FLAG2,S43,S54,S91
18 COUNTA = 2
19 R = 1.9858D0
20 C cal/mol/K
21 DATA C, SUM, DELTAT/0.0D0, 0.0D0, 0.0D0/
22 DATA TEMP, TT, Z/0.0D0, 0.0D0, 0.0D0/
23 ******************************************************
24 C
25 C INTRODUCTION
26 C
27 WRITE(6,101)
28 WRITE(6,51)
29 READ(5,*) (DAT(I),I=1,10)
30 IF (ADD(DAT).EQ.0.0D0) THEN
31 WRITE(6,159)
32 ELSE
33 WRITE(6,160)
34 IF (DAT(1).NE.0.0D0) WRITE(6,161)DAT(1)
35 IF (DAT(2).NE.0.0D0) WRITE(6,162)DAT(2)
36 IF (DAT(3).NE.0.0D0) WRITE(6,163)DAT(3)
37 IF (DAT(4).NE.0.0D0) WRITE(6,164)DAT(4)
38 IF (DAT(5).NE.0.0D0) WRITE(6,165)DAT(5)
```

```
39 IF (DAT(6).NE.0.0D0) WRITE(6,166)DAT(6)
40 IF (DAT(7).NE.0.0D0) WRITE(6,167)DAT(7)
41 IF (DAT(8).NE.0.0D0) WRITE(6,168)DAT(8)
42 IF (DAT(9).NE.0.0D0) WRITE(6,169)DAT(9)
43 IF (DAT(10).NE.0.0D0) WRITE(6,170)DAT(10)
44 ENDIF
45 WRITE(6,51)
46 101 FORMAT(1X,76(1H-),/,
47 1' Peritectic program by A. A. B. Sugden.',/,
48 2' This program calculates the phase boundaries of a given low allo
49 3y steel from',/,
50 4' 0 up to 5wt%C at appropriate intervals. This is done using the t
51 5hermodynamic',/,
52 6' formulae developed by Kirkaldy, Thomson, et al. Partition coeffi
53 7cients for',/,
54 8' the liquidus line are given for carbon and the solute elements.
55 9')
56 159 FORMAT(' Pure iron')
57 160 FORMAT(' The steel contains:')
58 161 FORMAT(F5.2,' wt% manganese')
59 162 FORMAT(F5.2,' wt% silicon')
60 163 FORMAT(F5.2,' wt% nickel')
61 164 FORMAT(F5.2,' wt% chromium')
62 165 FORMAT(F5.2,' wt% molybdenum')
63 166 FORMAT(F5.2,' wt% copper')
64 167 FORMAT(F5.2,' wt% vanadium')
65 168 FORMAT(F5.2,' wt% niobium')
66 169 FORMAT(F5.2,' wt% tungsten')
67 170 FORMAT(F5.2,' wt% cobalt')
68 ********************************************************
69 C
70 C MAIN PROGRAM
71 C
72 DO 19 MM = 1,9
73 C
74 C 1ST LOOP
75 C
76 K=MM
77 IF (K.EQ.2 .OR. K.EQ.8) GOTO 19
```

```
78 IF (K.GT.1) WRITE(6,51)
79 IF (K.GT.6) COUNT = 789
80 CALL FIRST(K)
81 DO 1 I = 1,10
82 1 XX(I) = DAT(I)
83 DUMMY = 0
84 2 C6 = 0.0D0
85 NUM = 0
86 C
87 C INITIALIZATION FOR K = 6
88 C
89 IF (COUNT.EQ.-1 .AND. DUMMY.EQ.0) K = 6
90 COUNT = 0
91 FLAG2 = 1
92 DTGAM = 0.0D0
93 Z61 = 1.0D2
94
95 IF (K.EQ.4) THEN
96 S43 = 3
97 K = K - 1
98 ENDIF
99
100 IF (K.EQ.7) THEN
101 CLIQ = -1.0D0
102 K = K - 6
103 ELSE
104 CLIQ = 5.3D-1
105 ENDIF
106
107 IF (K.EQ.9) THEN
108 S91 = 3
109 K = K - 2
110 GOTO 2
111 ENDIF
112
113 IF (S54.EQ.3) GOTO 3
114 IF (DUMMY.NE.3) THEN
115 IF (K.NE.5) WRITE(6,52)
116 IF (K.NE.6 .AND. K.NE.5) WRITE(6,55)
```

```
117 ENDIF
118 3 CONTINUE
119 DO 17 N = 1,70
120 C
121 C 2ND LOOP
122 C
123 IF (COUNT.EQ.-1 .OR. COUNT.EQ.12) GOTO 17
124 IF (K.EQ.5 .AND. NUM.EQ.3) GOTO 17
125 C = (N-1)*0.01
126 4 CONTINUE
127 IF (K.EQ.3 .OR. NUM.EQ.1) C = C*0.1
128 5 WTPC = C + ADD(XX)
129 IF (WTPC.GT.5.0) THEN
130 WRITE(6,52)
131 WRITE(6,54)
132 GOTO 18
133 ENDIF
134 C
135 C CALCULATION OF MOLE FRACTIONS
136 C
137 FEAF = (1.0D2-WTPC)/5.58D1
138 CAF = C/1.2D1
139 DO 6 M = 1,10
140 6 X(M) = XX(M)/B(M,1)
141 TAF = FEAF + CAF + ADD(X)
142 CF = CAF/TAF
143 DO 7 M = 1,10
144 7 X(M) = X(M)/TAF
145
146 IF (K.EQ.1) THEN
147 IF (C.LE.CLIQ) THEN
148 IF (NUM.EQ.1) THEN
149 TO = 1.809D3 - 2.013D2*C - 2.949D3*C*C
150 ELSE
151 TO = 1.809D3 - 2.956D1*C - 8.6D1*C*C
152 ENDIF
153 H = 3.3D3
154 C cal/mol
155 HC = -2.13D4
```

```
156 T = TO
157 8 CONTINUE
158 GC = 6.3D0*T - 2.13D4
159 GOTO 10
160 ELSE
161 IF (S91.EQ.3) THEN
162 TO = 1.783D3 - 1.640D2*C - 1.674D1*C*C
163 ELSE
164 TO = 1.799D3 - 5.432D1*C - 7.869D0*C*C
165 ENDIF
166 T = TO
167 H = 3.6D3
168 HC = -5.36D3
169 9 CONTINUE
170 GC = 6.0D-1*T - 5.36D3
171 ENDIF
172 10 AC = DEXP(GC/(R*TO)+(3.89D-1+7.81D3/T)*CF)
173 AC = AC/(1+(8.91D3/T)*CF*DEXP(GC/(R*TO)))
174 ENDIF
175
176 IF (K.EQ.3) THEN
177 IF (DUMMY.EQ.0) THEN
178 K = K + 3
179 DUMMY = 3
180 GOTO 5
181 ENDIF
182 DUMMY = 8
183 IF (S43.EQ.3) THEN
184 TO = 1.667D3 + 1.122D3*C
185 C
186 C REF: METALS HANDBOOK, 1978
187 C
188 ELSE
189 TO = 1.667D3 + 9.81D2*C - 2.17D3*C*C
190 ENDIF
191 H = 2.0D2
192 HC = -1.5325D4
193 T = TO
194 CF = 0
```

```
195 12 G = -1.36D-1*T + 2.258D2
196 GC = -7.686D0*T + 1.5325D4
197 ENDIF
198
199 IF (K.EQ.5) THEN
200 IF (DUMMY.EQ.0 .AND. COUNT.NE.11) THEN
201 K = K + 1
202 DUMMY = 5
203 GOTO 5
204 ENDIF
205 DUMMY = -1
206 K = K - 4
207 NUM = NUM + 1
208 GOTO 5
209 ENDIF
210
211 IF (K.EQ.6) THEN
212 K = K - 5
213 C = CLIQ
214 COUNT = 3
215 GOTO 5
216 13 IF (DELTAT.EQ.0.0D0) THEN
217 COUNT = -1
218 GOTO 15
219 ELSE
220 FLAG1 = COUNT/COUNTA
221 IF (FLAG1.NE.FLAG2) THEN
222 DTGAM = DELTAT
223 IF (DELTAT.GT.0.0D0) THEN
224 CLIQ = CLIQ - 5.0D-3
225 ELSE
226 CLIQ = CLIQ + 5.0D-3
227 ENDIF
228 C = CLIQ
229 ELSE
230 DTALPH = DELTAT
231 C = CLIQ + 1.0D-3
232 ENDIF
233 Z6 = DTALPH - DTGAM
```

```
234 Z6 = DABS(Z6)
235 IF (Z6.GT.Z61) THEN
236 T = T - Z6
237 COUNT = -1
238 GOTO 15
239 ENDIF
240 COUNT = COUNT + 1
241 FLAG2 = FLAG1
242 Z61 = Z6
243 GOTO 5
244 ENDIF
245 ENDIF
246
247 SUM = 0.0D0
248 DELTAT = 0.0D0
249 DO 14 M = 1,10
250 C
251 C 3RD LOOP
252 C
253 IF (X(M).EQ.0) THEN
254 A(M)=0.0D0
255 AI(M)=1.0D0
256 GOTO 14
257 ENDIF
258
259 IF (K.EQ.1) THEN
260 IF (C.LE.CLIQ) THEN
261 Q = 0.0D0
262 ELSE
263 Q = B(M,4) + B(M,5)/T
264 ENDIF
265 P = B(M,2) + B(M,3)/T
266 IF (C.LE.CLIQ) THEN
267 G = -2646+39.1693*T-5.27*T*DLOG(T)+0.001*T*T-0.136*T+2.258D2
268 GI = -(D(M,5) + D(M,6)*T)
269 ELSE
270 G = - 2646 + 39.1693*T - 5.27*T*DLOG(T) + 0.001*T*T
271 GI = -(D(M,1) + (D(M,2) + D(M,3)*DLOG(T) + D(M,4)*T)*T)
272 ENDIF
```

```
C
C CALCULATION OF SOLUTE PARTITION COEFFICIENTS FOR THE LIQUIDUS
C
AI(M) = DEXP(GI/(R*TO)+P*CF)
AI(M) = AI(M)/(1+Q*CF*DEXP(GC/(R*TO)))
ENDIF

IF (K.EQ.3) THEN
P = 0.0D0
Q = B(M,4) + B(M,5)/T
IF (M.EQ.1) THEN
GI = 6.5D2 - 3.05D-1*T
ELSE
IF (M.EQ.3) THEN
GI = 3.0D2
ELSE
IF (M.EQ.6) THEN
GI = 1.45D3 - 8.0D-1*T
ELSE
GI = -(E(M,1)+(E(M,2)+E(M,3)*T+E(M,4)*DLOG(T))*T)
C
C NOTE MINUS SIGN
C
ENDIF
ENDIF
ENDIF
ENDIF

CALL EQN(A(M),K,C,CLIQ)
SUM = SUM + X(M)*A(M)
14 CONTINUE
DELTAT = SUM*R*TO*TO
T = TO + DELTAT
Z = TT - T
Z = DABS(Z)
IF (Z.LT.0.5D0) GOTO 15
TT = T
IF (K.EQ.1) THEN
IF (C.LE.CLIQ) THEN
```

```
312 GOTO 8
313 ELSE
314 GOTO 9
315 ENDIF
316 ENDIF
317 IF (K.EQ.3) GOTO 12
318 15 CONTINUE
319
320 IF (K.EQ.3) THEN
321 IF (T.GT.TEMP) THEN
322 IF (COUNT.EQ.0) THEN
323 C = (N-1)*0.02 - 0.01
324 COUNT = 11
325 GOTO 5
326 ELSE
327 IF (NUM.NE.2) THEN
328 WRITE(6,52)
329 IF (S43.EQ.3) THEN
330 WRITE(6,59)C-5.0D-3
331 ELSE
332 WRITE(6,58)C-5.0D-3
333 ENDIF
334 IF (DUMMY.EQ.8) THEN
335 WRITE(6,60)TEMP-273
336 ELSE
337 WRITE(6,60)TEMP
338 ENDIF
339 COUNT = 12
340 GOTO 17
341 ENDIF
342 ENDIF
343 ELSE
344 IF (COUNT.EQ.11) THEN
345 IF (NUM.NE.2) THEN
346 WRITE(6,52)
347 IF (S43.EQ.3) THEN
348 WRITE(6,59)C+5.0D-3
349 ELSE
350 WRITE(6,58)C+5.0D-3
```

```
351 ENDIF
352 IF (DUMMY.EQ.8) THEN
353 WRITE(6,60)TEMP-273
354 ELSE
355 WRITE(6,60)TEMP
356 ENDIF
357 COUNT = 12
358 GOTO 17
359 ENDIF
360 ENDIF
361 ENDIF
362 ENDIF
363
364 IF (COUNT.GE.3) GOTO 13
365 IF (COUNT.EQ.-1)THEN
366 IF (DUMMY.EQ.0) THEN
367 WRITE(6,60)T-273
368 WRITE(6,61)C
369 ELSE
370 TEMP = T
371 ENDIF
372 GOTO 17
373 ENDIF
374 IF (K.EQ.3 .AND. S54.EQ.3) GOTO 17
375 IF (K.EQ.3 .AND. S93.NE.3) THEN
376 IF (NUM.NE.2) THEN
377 WRITE(6,62)C,T-273
378 ELSE
379 WRITE(6,63)C,T-273
380 ENDIF
381 ELSE
382 IF (S91.EQ.3 .AND. N.EQ.1) GOTO 17
383 IF (NUM.EQ.1) THEN
384 IF (T.LT.TEMP) THEN
385 WRITE(6,52)
386 WRITE(6,57)
387 COUNT = -1
388 GOTO 17
389 ELSE
```

```
390 WRITE(6,62)C,T-273
391 ENDIF
392 ELSE
393 C
394 C K = 1
395 C
396 WRITE(6,63)C,T-273
397 IF (K.EQ.1) THEN
398 IF (CLIQ.EQ.-1.0D0 .OR. S91.EQ.3) GOTO 17
399 WRITE(6,64)AC
400 DO 16 I = 1,10
401 IF (AI(I).EQ.1.0D0) GOTO 16
402 IF (I.LT.9) THEN
403 WRITE(6,65)I+1,AI(I)
404 ELSE
405 WRITE(6,66)I+1,AI(I)
406 ENDIF
407 16 CONTINUE
408 ENDIF
409 ENDIF
410 ENDIF
411 17 CONTINUE
412 IF (K.EQ.1 .OR. K.EQ.5) THEN
413 IF (DUMMY.EQ.-1) GOTO 18
414 ENDIF
415 IF (DUMMY.NE.0 .AND. DUMMY.NE.8) THEN
416 IF (DUMMY.EQ.3) K = K + 2
417 IF (DUMMY.EQ.5) K = K + 4
418 GOTO 2
419 ENDIF
420 18 CONTINUE
421 19 CONTINUE
422 STOP
423
424 51 FORMAT(1X,63(1H-))
425 52 FORMAT(1X)
426 54 FORMAT(' The sum of the alloy components should not exceed 5wt%')
427 55 FORMAT(' WT%C : T/Centigrade')
428 57 FORMAT(' Solidus ends.')
```

```
429 58 FORMAT(' The peritectic point is at ',F4.2,' wt%C.')
430 59 FORMAT(' The maximum solubility of the carbon in delta-iron is ',F
431 14.2,' wt%.')
432 60 FORMAT(' The peritectic line is at approx. ',F6.1,' Centigrade')
433 61 FORMAT(' The line stops at ',F5.3,' wt%C.')
434 62 FORMAT(' ',F6.3,' ',F6.1)
435 63 FORMAT(' ',F6.4,' ',F6.1)
436 64 FORMAT(' A(c):',F6.3)
437 65 FORMAT(' A(',I1,'):',F6.3)
438 66 FORMAT(' A(',I2,'):',F6.3)
439 END
440
441 C
442 C DATA FOR ALLOYING ELEMENT INTERACTION PARAMETERS
443 C
444 BLOCK DATA ETA
445 COMMON /INTER/B
446 DOUBLE PRECISION B(10,5)
447 DATA((B(M,J),J=1,5),M=1,10)/
448 C5.49D1,0.0D0,-5.06D3,0.0D0,-5.07D3,
449 C2.81D1,-4.28D-1,1.874D4,4.84D0,-7.37D3,
450 C5.87D1,0.0D0,5.34D3,-2.2D0,7.6D3,
451 C5.20D1,0.0D0,-9.5D3,2.44D1,-3.84D4,
452 C9.59D1,0.0D0,-7.49D3,3.855D0,-1.787D4,
453 C6.35D1,0.0D0,7.586D3,0.0D0,4.2D3,
454 C5.09D1,0.0D0,-3.01D4,0.0D0,-2.466D4,
455 C9.29D1,0.0D0,-4.6615D4,0.0D0,-2.877D4,
456 C1.838D2,0.0D0,-1.223D4,2.34D1,-3.6214D4,
457 C5.89D1,0.0D0,3.55D3,0.0D0,2.8D3/
458 END
459
460 C
461 C DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))
462 C [LIQUID-AUSTENITE AND LIQUID-FERRITE TRANSFORMATIONS]
463 C
464 BLOCK DATA DGI1
465 COMMON /DELTA1/ D
466 DOUBLE PRECISION D(10,6)
467 DATA ((D(M,J),J=1,6),M=1,10)/
```

```
468 C-2.86D3,2.03D0,0.0D0,0.0D0,-2213.0D0,1.727D0,
469 C2.236D3,3.49D1,-4.7244D0,0.0D0,8.2D3,-3.9D0,
470 C7.9D2,6.4D-1,0.0D0,0.0D0,2.12D3,3.8D-1,
471 C4.233D3,-6.89D0,6.568D-1,0.0D0,4.6D3,-2.19D0,
472 C7.165D3,-2.14D0,0.0D0,0.0D0,6.6D3,-2.29D0,
473 C3.15D3,-1.39D0,0.0D0,0.0D0,1.2D3,0.0D0,
474 C-3.257D3,1.15D1,0.0D0,-5.1D-3,5.1D3,-2.3D0,
475 C5.5D3,-2.3D0,0.0D0,0.0D0,5.5D3,-2.3D0,
476 C1.0D4,-3.5D0,0.0D0,0.0D0,7.5D3,-3.65D0,
477 C-3.95D3,2.19D0,0.0D0,0.0D0,-3.5D3,2.19D0/
478 END
479
480 C
481 C DATA FOR ALLOYING ELEMENT FREE ENERGY CHANGES (DELTA G(I))
482 C [FERRITE-AUSTENITE TRANSFORMATION]
483 C
484 BLOCK DATA DGI2
485 COMMON /DELTA2/E
486 DOUBLE PRECISION E(10,4)
487 DATA((E(M,J),J=1,4),M=1,10)/
488 C-1.76D3,-4.7D-1,0.0D0,0.0D0,
489 C-5.964D3,3.8799D1,0.0D0,-4.7244D0,
490 C-5.607D3,-3.8D-1,0.0D0,0.0D0,
491 C-3.67D2,-4.656D0,0.0D0,6.568D-1,
492 C5.65D2,1.5D-1,0.0D0,0.0D0,
493 C-2.55D4,4.1183D1,-1.7D-1,0.0D0,
494 C-8.357D3,1.38D1,-5.1D-3,0.0D0,
495 C1.434D1,-1.3D-3,0.0D0,0.0D0,
496 C2.5D3,1.5D-1,0.0D0,0.0D0,
497 C0.0D0,0.0D0,0.0D0,0.0D0/
498 END
499
500 SUBROUTINE FIRST(L)
501 IF (L.EQ.1) WRITE(6,1)
502 IF (L.EQ.3) WRITE(6,3)
503 IF (L.EQ.4) WRITE(6,4)
504 IF (L.EQ.5) WRITE(6,5)
505 IF (L.EQ.6) WRITE(6,6)
506 IF (L.EQ.7) WRITE(6,7)
```

```
507 IF (L.EQ.9) WRITE(6,9)
508 RETURN
509 1 FORMAT (' Liquidus.')
510 3 FORMAT (' Austenite/Delta+Austenite line.')
511 4 FORMAT (' Delta/Delta+Austenite line.')
512 5 FORMAT (' Delta solidus.')
513 6 FORMAT (' Peritectic line.')
514 7 FORMAT (' Solidification as primary austenite.')
515 9 FORMAT (' Austenite solidus.')
516 END
517
518 DOUBLE PRECISION FUNCTION ADD(Y)
519 DOUBLE PRECISION Y(10)
520 ADD = 0.0D0
521 DO 4 I = 1,10
522 4 ADD = ADD + Y(I)
523 RETURN
524 END
525 ************************************************
526 C
527 C MAIN CALCULATION
528 C
529 SUBROUTINE EQN (F16,NO,CC,CQIL)
530 IMPLICIT DOUBLE PRECISION (F)
531 DOUBLE PRECISION G,R,TO,T,P,CF,Q,GC,GI,HC,H
532 DOUBLE PRECISION CC,CQIL,EG11,EL11
533 COMMON /PARMS/G,R,TO,T,P,CF,Q,GC,GI,HC,H
534 C
535 C SET CARBON-CARBON INTERACTION PARAMETERS
536 C
537 IF (NO.EQ.1) THEN
538 IF (CC.LE.CQIL) THEN
539 EG11 = 0.0D0
540 ELSE
541 EG11 = 8.91D3/T
542 ENDIF
543 EL11 = 3.89D-1 + 7.81D3/T
544 ENDIF
545 IF (NO.EQ.2) THEN
```

```
546 EG11 = 0.0D0
547 EL11 = 8.91D3/T
548 ENDIF
549 IF (NO.EQ.3) THEN
550 EG11 = 8.91D3/T
551 EL11 = 0.0D0
552 ENDIF
553 F1 = GI/(R*TO) + P*CF
554 F2 = GC/(R*TO)
555 F3 = 1 + Q*CF*DEXP(F2)
556 F4 = GC/(R*TO) + (EL11)*CF
557 F5 = 1 + EG11*CF*DEXP(F2)
558 F6 = DEXP(F1)/F3
559 F7 = DEXP(F4)/F5
560 F8 = 1+CF*(1-CF)*(P-Q*F6*F7)
561 F9 = G/(R*TO*TO)
562 F10 = CF*CF/2*((EL11)-(EG11*F7*F7))
563 F11 = DEXP(F4)*CF*HC/F5
564 F12 = (1-CF)*H
565 F13 = F9 - F10
566 F14 = F11+F12*DEXP(F13)
567 F15 = F8*DEXP(F13)
568 F16 = (F6-F15)/F14
569 RETURN
570 END
571 %
```

APPENDIX 4: STRENGTHENING PROGRAM

```
1 FTVSCLR PROGRAM=%H% DATA=.DATA NAG OUTPUT=.OUT:TWO
2 C
3 C PROGRAM TO CALCULATE SOLID SOLUTION STRENGTHENING
4 C AND STRENGTHENING DUE TO PURE ANNEALED IRON
5 C AS A FUNCTION OF TEMPERATURE AND STRAIN RATE.
6 C COPYRIGHT A. A. B. SUGDEN 1987.
7 C REF: SUGDEN AND BHADESHIA, METALL. TRANS. A., 19A, 1597-1603.
8 C ENTER THE FOLLOWING VARIABLES (COMPOSITIONS IN WT%):
9 C TEMPERATURE, Ni, Mn, Si, Cr, Co, V, Ti.
10 C Mo, Al, Nb, XX, P, C, N, B, STRAIN RATE,
11 C TEMPERATURE RANGE: 100 TO 750K.
12 C STRAIN RATE RANGE: 5X10-6 TO 10-2/S (AN APPROPRIATE DEFAULT
13 C SETTING IS CHOSEN).
14 C XX IS A DUMMY VARIABLE, AND MEANS THAT ANOTHER ELEMENT MAY
BE
15 C ADDED VERY EASILY.
16 C
17 IMPLICIT REAL*8(A-H,O-$)
18 DOUBLE PRECISION BLOCK(20,500)
19 DIMENSION C(15),DAT(15),DELSIG(15),NUM(15),Q(15)
20 DIMENSION TTLSUM(500),YLDSTR(500)
21 COMMON/TOT/TTLSUM
22 COMMON/PARM/SRATE
23 COMMON/PARMS/C,DAT,T
24 DATA DELSIG(12), DS, P/0.0D0, 0.0D0, 0.0D0/
25 DATA Q/15*0.0D0/,NUM/15*0/
26
27 READ(5,*) I21,((BLOCK(J,I),J=1,20),I=1,I21)
28 DO 88 I22 = 1,I21
29 T = BLOCK(1,I22)
30 DO 77 I23 = 2,16
31 N = I23 - 1
32 77 DAT(N) = BLOCK(I23,I22)
33 SRATE = BLOCK(17,I22)
34 T = T + 2.73D2
35 CALL ATOMFR
36 CALL IFDS(C,DELSIG,NUM)
37 CALL ELSEDS(Q)
```

```
38 IF (DAT(12).GT.0.0D0) CALL PHOS(C(12),DELSIG(12),NUM(12))
39 CALL RESULT(DELSIG,Q,NUM,I22)
40 WRITE(6,101)
41 YLDSTR(I22) = (BLOCK(18,I22)*9.80665D0)/3.0D0
42 C
43 C CALCULATION OF YIELD STRENGTH FROM HARDNESS
44 C
45 CALL NCALC(YLDSTR(I22), BLOCK(19,I), BLOCK(20,I))
46 88 CONTINUE
47 WRITE(6,105)I21
48 DO 4 I = 1,I21
49 $MICRO = YLDSTR(I) - TTLSUM(I)
50 4 WRITE(6,110)BLOCK(18,I),YLDSTR(I),TTLSUM(I),
51 &$MICRO,BLOCK(19,I)/1.0D2,BLOCK(20,I)/1.0D2
52 STOP
53 101 FORMAT(1X,50(1H*))
54 105 FORMAT(' SUMMARY:',/,
55 &' HV TOTAL/MPA SS+FE/MPA MICRO/MPA VALPHA VACIC
56 &SETS OF DATA',/,
57 &' ————————Delete the above for regression analysis——
58 &————————',/,
59 &'
60 & ',I3)
61 110 FORMAT(F8.2,2F12.2,F10.2,2F10.4)
62 END
63 ************************************************************************
64 SUBROUTINE ATOMFR
65 C
66 C CALCULATES ATOM FRACTIONS OF THE ALLOYING ELEMENTS
67 C
68 DOUBLE PRECISION AW(15),C(15),DAT(15),FEAF,T,TAF
69 COMMON/PARMS/C,DAT,T
70 DATA AW(1),AW(2),AW(3)/5.87D1,5.49D1,2.81D1/,
71 * AW(4),AW(5),AW(6),AW(7)/5.2D1,5.89D1,5.09D1,4.79D1/,
72 * AW(8),AW(9),AW(10),AW(11)/9.59D1,2.7D1,9.3D1,1.0D2/,
73 * AW(12),AW(13),AW(14),AW(15)/3.1D1,1.2D1,1.4D1,1.08D1/
74 DO 4 I = 1,15
75 4 C(I) = DAT(I)/AW(I)
76 FEAF = (1.0D2-ADD(DAT))/5.58D1
```

```
77 TAF = FEAF + ADD(C)
78 DO 6 I = 1,15
79 6 C(I) = C(I)*1.0D2/TAF
80 END
81 ************************************************************************
82 FUNCTION ADD(Y)
83 DOUBLE PRECISION Y(15)
84 ADD = 0.0D0
85 DO 4 I = 1,15
86 4 ADD = ADD + Y(I)
87 RETURN
88 END
89 ************************************************************************
90 SUBROUTINE IFDS(AT,DSI,I1)
91 C
92 C CALCULATES STRENGTHENING DUE TO NI, MN, SI, CR, CO, V, TI, MO, AL,
93 C NB AND XX AT 23 DEGC
94 C
95 DOUBLE PRECISION AT(15),DSI(15),FACTOR(11),LIM(11)
96 INTEGER I1(15)
97 DATA FACTOR(1),FACTOR(2),FACTOR(3)/1.965D1,1.85D1,2.68D1/,
98 * FACTOR(4),FACTOR(5),FACTOR(6)/3.5D0,3.43D0,2.07D0/,
99 * FACTOR(7),FACTOR(8),FACTOR(9)/1.76D1,1.55D1,9.31D0/
100 * FACTOR(10),FACTOR(11),LIM(1),LIM(2)/0.0D0,0.0D0,2.84D0,2.97D0/,
101 * LIM(3),LIM(4),LIM(5),LIM(6)/5.72D0,6.86D0,5.56D0,1.043D1/,
102 * LIM(7),LIM(8),LIM(9),LIM(10)/1.0D1,1.79D0,5.85D0,1.0D1/,
103 * LIM(11)/1.0D1/
104 C
105 C LIMITS FOR TI AND NB SET AT 10%
106 C
107 DO 5 I = 1,11
108 DSI(I) = FACTOR(I)*AT(I)
109 5 IF (AT(I).GT.LIM(I)) I1(I) = 1
110 END
111 ************************************************************************
112 SUBROUTINE ELSEDS(ELSE)
113 C
114 C CALCULATES STRENGTHENING DUE TO NI, MN, SI, CR, AND CO AT
115 C T.NE.23DEGC
```

```
116 C
117 DOUBLE PRECISION C(15),DAT(15),T,ELSE(15)
118 COMMON/PARMS/C,DAT,T
119 IF (DAT(1).GT.0.0D0) CALL NICKEL(C(1),T,ELSE(1))
120 IF (DAT(2).GT.0.0D0) CALL MANGAN(C(2),T,ELSE(2))
121 IF (DAT(3).GT.0.0D0) CALL SILICN(C(3),T,ELSE(3))
122 IF (DAT(4).GT.0.0D0) CALL CHROM(C(4),T,ELSE(4))
123 IF (DAT(5).GT.0.0D0) CALL COBALT(C(5),T,ELSE(5))
124 END
125 ************************************************************************
126 SUBROUTINE NICKEL(CONC,XARG,DNI)
127 DOUBLE PRECISION K(13),KNI(2,13),C(13),CNI(2,13)
128 DOUBLE PRECISION X(2),Y(2),A1,A2,DNI
129 DATA CNI(1,1),CNI(1,2),CNI(1,3)/-3.86D1,-4.67D1,-6.8D1/,
130 * CNI(1,5),CNI(1,6),CNI(1,7),CNI(1,8)/6.57D1,2.8D1,3.61D1,1.45D1/,
131 * CNI(1,9),CNI(1,10),CNI(1,11),CNI(1,12)/1.62D1,0.0D0,0.0D0,0.0D0/
132 * ,CNI(1,13),CNI(2,1),CNI(2,2)/0.0D0,-5.7D1,-4.8D1/,
133 * CNI(2,4),CNI(2,5),CNI(2,6),CNI(2,7)/6.38D1,1.39D2,7.9D1,7.56D1/,
134 * CNI(2,8),CNI(2,9),CNI(2,10),CNI(2,11)/4.03D1,3.91D1,0.0D0,0.0D0/
135 * ,CNI(2,12),CNI(2,13),KNI(1,1),KNI(1,2)/0.0D0,0.0D0,1.0D2,1.0D2/,
136 * KNI(1,3),KNI(1,4),KNI(1,5),KNI(1,6)/1.0D2,1.0D2,1.6D2,2.1D2/,
137 * KNI(1,7),KNI(1,8),KNI(1,9),KNI(1,10)/2.5D2,3.4D2,5.8D2,7.5D2/,
138 * KNI(1,11),KNI(1,12),KNI(1,13),KNI(2,1)/7.5D2,7.5D2,7.5D2,1.0D2/,
139 * KNI(2,2),KNI(2,3),KNI(2,4),KNI(2,5)/1.0D2,1.0D2,1.0D2,1.7D2/,
140 * KNI(2,6),KNI(2,7),KNI(2,8),KNI(2,9)/2.1D2,2.6D2,4.25D2,6.0D2/,
141 * KNI(2,10),KNI(2,11),KNI(2,12),KNI(2,13)/7.5D2,7.5D2,7.5D2,7.5D2/
142 * ,CNI(1,4),CNI(2,3)/-3.5D1,-1.17D2/
143 DATA NCAP7,IFAIL/13,0/
144 DATA X(1),X(2)/1.44D0,2.84D0/
145 C
146 C CALCULATE DNI AT A GIVEN TEMPERATURE FOR TWO CONCENTRATIONS
147 C
148 DO 8 I = 1,2
149 DO 5 J = 1,13
150 K(J) = KNI(I,J)
151 5 C(J) = CNI(I,J)
152 8 CALL E02BBF(NCAP7,K,C,XARG,Y(I),IFAIL)
153 C
154 C EXPRESS DNI AS A FUNCTION OF CONCENTRATION
```

```
C
A2 = (Y(2)/X(2)-Y(1)/X(1))/(X(2)-X(1))
A1 = Y(1)/X(1) - A2*X(1)
DNI = A1*CONC + A2*CONC*CONC
END
************************************************************************
SUBROUTINE MANGAN(CONC,XARG,DMN)
DOUBLE PRECISION K(13),KMN(2,13),C(13),CMN(2,13)
DOUBLE PRECISION X(2),Y(2),A1,A2,DMN
DATA CMN(1,1),CMN(1,2),CMN(1,3)/-1.25D1,-6.22D1,-5.16D1/,
* CMN(1,4),CMN(1,5),CMN(1,6)/-1.01D2,7.02D1,5.66D1/,
* CMN(1,7),CMN(1,8),CMN(1,9)/5.12D1,3.07D1,2.585D1/,
* CMN(1,10),CMN(1,11),CMN(1,12),CMN(1,13)/0.0D0,0.0D0,0.0D0,0.0D0/,
* KMN(1,1),KMN(1,2),KMN(1,3),KMN(1,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
* KMN(1,5),KMN(1,6),KMN(1,7),KMN(1,8)/1.3D2,1.9D2,2.3D2,3.2D2/,
* KMN(1,9),KMN(1,10),KMN(1,11)/5.6D2,7.5D2,7.5D2/,
* KMN(1,12),KMN(1,13)/7.5D2,7.5D2/
DATA CMN(2,1),CMN(2,2),CMN(2,3)/-5.02D1,-4.975D1,-1.46D2/,
* CMN(2,4),CMN(2,5),CMN(2,6)/9.02D1,1.135D2,6.94D1/,
* CMN(2,7),CMN(2,8),CMN(2,9)/6.95D1,6.905D1,6.17D1/,
* CMN(2,10),CMN(2,11),CMN(2,12),CMN(2,13)/0.0D0,0.0D0,0.0D0,0.0D0/
* ,KMN(2,1),KMN(2,2),KMN(2,3),KMN(2,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
* KMN(2,5),KMN(2,6),KMN(2,7),KMN(2,8)/1.625D2,2.0D2,3.0D2,4.875D2/
* KMN(2,9),KMN(2,10),KMN(2,11)/6.5D2,7.5D2,7.5D2/,
* KMN(2,12),KMN(2,13)/7.5D2,7.5D2/
DATA NCAP7,IFAIL/13,0/
DATA X(1),X(2)/1.54D0,2.97D0/
DO 8 I = 1,2
DO 5 J = 1,13
K(J) = KMN(I,J)
5 C(J) = CMN(I,J)
8 CALL E02BBF(NCAP7,K,C,XARG,Y(I),IFAIL)
A2 = (Y(2)/X(2)-Y(1)/X(1))/(X(2)-X(1))
A1 = Y(1)/X(1) - A2*X(1)
DMN = A1*CONC + A2*CONC*CONC
END
************************************************************************
SUBROUTINE SILICN(CONC,XARG,DSI)
DOUBLE PRECISION K(13),KSI(3,13),C(13),CSI(3,13),FIT,XARG
```

```
194 DOUBLE PRECISION X(4),Y(4),W(4),WORK1(3,4),WORK2(2,3)
195 DOUBLE PRECISION A(3,3),S(3),B(3),CONC,DSI,XCAP
196 INTEGER M,KPLUS1,NROWS,IFAIL,NPLUS1
197 DATA CSI(1,1),CSI(1,2),CSI(1,3)/-3.575D1,-7.84D1,-3.97D1/,
198 * CSI(1,4),CSI(1,5),CSI(1,6)/-1.245D2,5.53D1,7.71D1/,
199 * CSI(1,7),CSI(1,8),CSI(1,9)/4.75D1,5.205D1,4.04D1/
200 * CSI(1,10),CSI(1,11),CSI(1,12),CSI(1,13)/0.0D0,0.0D0,0.0D0,0.0D0/
201 * ,KSI(1,1),KSI(1,2),KSI(1,3),KSI(1,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
202 * KSI(1,5),KSI(1,6),KSI(1,7),KSI(1,8)/1.3D2,1.8D2,2.3D2,2.9D2/,
203 * KSI(1,9),KSI(1,10),KSI(1,11)/4.6D2,7.5D2,7.5D2/,
204 * KSI(1,12),KSI(1,13)/7.5D2,7.5D2/
205 DATA CSI(2,1),CSI(2,2),CSI(2,3)/-3.69D1,-4.93D0,-1.06D2/,
206 * CSI(2,4),CSI(2,5),CSI(2,6)/1.065D2,1.795D2,9.54D1/,
207 * CSI(2,7),CSI(2,8),CSI(2,9)/1.205D2,8.37D1,9.255D1/,
208 * CSI(2,10),CSI(2,11),CSI(2,12),CSI(2,13)/0.0D0,0.0D0,0.0D0,0.0D0/
209 * ,KSI(2,1),KSI(2,2),KSI(2,3),KSI(2,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
210 * KSI(2,5),KSI(2,6),KSI(2,7),KSI(2,8)/1.3D2,2.0D2,2.75D2,4.125D2/,
211 * KSI(2,9),KSI(2,10),KSI(2,11),KSI(2,12)/6.0D2,7.5D2,7.5D2,7.5D2/,
212 * KSI(2,13)/7.5D2/
213 DATA CSI(3,1),CSI(3,2),CSI(3,3)/8.87D1,1.39D2,2.41D2/,
214 * CSI(3,4),CSI(3,5),CSI(3,6)/3.28D2,3.04D2,2.5D2/,
215 * CSI(3,7),CSI(3,8),CSI(3,9)/2.15D2,1.79D2,1.68D2/,
216 * CSI(3,10),CSI(3,11),CSI(3,12),CSI(3,13)/0.0D0,0.0D0,0.0D0,0.0D0/
217 * ,KSI(3,1),KSI(3,2),KSI(3,3),KSI(3,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
218 * KSI(3,5),KSI(3,6),KSI(3,7),KSI(3,8)/2.2D2,2.8D2,3.1D2,4.0D2/,
219 * KSI(3,9),KSI(3,10),KSI(3,11),KSI(3,12)/5.75D2,7.5D2,7.5D2,7.5D2/,
220 * KSI(3,13)/7.5D2/
221 DATA NCAP7,IFAIL/13,0/
222 DATA X(1),X(2),X(3),X(4),Y(1)/0.0D0,1.38D0,2.8D0,5.72D0,0.0D0/,
223 * W(1),W(2),W(3),W(4)/1.0D3,1.0D0,1.0D0,1.0D0/
224 DATA M,KPLUS1,NROWS,NPLUS1/4,3,3,3/
225 DO 8 I = 1,3
226 DO 5 J = 1,13
227 K(J) = KSI(I,J)
228 5 C(J) = CSI(I,J)
229 CALL E02BBF(NCAP7,K,C,XARG,FIT,IFAIL)
230 8 Y(I+1) = FIT
231 CALL E02ADF(M,KPLUS1,NROWS,X,Y,W,WORK1,WORK2,A,S,IFAIL)
232 DO 12 I = 1,3
```

```
233 12 B(I) = A(3,I)
234 XCAP = (2.0D0*CONC-X(4))/X(4)
235 CALL E02AEF(NPLUS1,B,XCAP,DSI,IFAIL)
236 END
237 ************************************************************************
238 SUBROUTINE CHROM(CONC,XARG,DCR)
239 DOUBLE PRECISION K(13),KCR(3,13),C(13),CCR(3,13),FIT,XARG
240 DOUBLE PRECISION X(4),Y(4),W(4),WORK1(3,4),WORK2(2,3)
241 DOUBLE PRECISION A(3,3),S(3),B(3),CONC,DCR,XCAP
242 INTEGER M,KPLUS1,NROWS,IFAIL,NPLUS1
243 DATA CCR(1,1),CCR(1,2),CCR(1,3)/3.47D1,2.815D1,4.1D1/,
244 * CCR(1,4),CCR(1,5),CCR(1,6),CCR(1,7)/-1.3D1,1.56D1,1.02D1,4.38D1/
245 * ,CCR(1,8),CCR(1,9),CCR(1,10)/5.21D0,1.6D0,0.0D0/,
246 * CCR(1,11),CCR(1,12),CCR(1,13),KCR(1,1)/0.0D0,0.0D0,0.0D0,1.0D2/,
247 * KCR(1,2),KCR(1,3),KCR(1,4),KCR(1,5)/1.0D2,1.0D2,1.0D2,1.7D2/,
248 * KCR(1,6),KCR(1,7),KCR(1,8),KCR(1,9)/2.1D2,2.6D2,3.0D2,4.8D2/,
249 * KCR(1,10),KCR(1,11),KCR(1,12)/7.5D2,7.5D2,7.5D2/,
250 * KCR(1,13)/7.5D2/
251 DATA CCR(2,1),CCR(2,2),CCR(2,3)/5.71D1,5.176D1,3.55D1/,
252 * CCR(2,4),CCR(2,5),CCR(2,6)/2.27D1,1.36D1,7.87D0/,
253 * CCR(2,7),CCR(2,8),CCR(2,9)/9.57D0,6.95D0,7.185D0/,
254 * CCR(2,10),CCR(2,11),CCR(2,12),CCR(2,13)/0.0D0,0.0D0,0.0D0,0.0D0/
255 * ,KCR(2,1),KCR(2,2),KCR(2,3),KCR(2,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
256 * KCR(2,5),KCR(2,6),KCR(2,7),KCR(2,8)/1.3D2,1.9D2,3.143D2,4.25D2/,
257 * KCR(2,9),KCR(2,10),KCR(2,11),KCR(2,12)/6.0D2,7.5D2,7.5D2,7.5D2/,
258 * KCR(2,13)/7.5D2/
259 DATA CCR(3,1),CCR(3,2),CCR(3,3)/1.08D-1,5.96D0,1.45D1/,
260 * CCR(3,4),CCR(3,5),CCR(3,6)/1.42D0,1.07D0,5.76D1/,
261 * CCR(3,7),CCR(3,8),CCR(3,9)/2.12D1,3.5D1,1.61D1/,
262 * CCR(3,10),CCR(3,11),CCR(3,12),CCR(3,13)/0.0D0,0.0D0,0.0D0,0.0D0/
263 * ,KCR(3,1),KCR(3,2),KCR(3,3),KCR(3,4)/1.0D2,1.0D2,1.0D2,1.0D2/,
264 * KCR(3,5),KCR(3,6),KCR(3,7),KCR(3,8)/1.5D2,2.1D2,2.3D2,2.8D2/,
265 * KCR(3,9),KCR(3,10),KCR(3,11)/3.3D2,7.5D2,7.5D2/,
266 * KCR(3,12),KCR(3,13)/7.5D2,7.5D2/
267 DATA NCAP7,IFAIL/13,0/
268 DATA X(1),X(2),X(3),X(4),Y(1)/0.0D0,1.65D0,3.1D0,6.86D0,0.0D0/,
269 * W(1),W(2),W(3),W(4)/1.0D3,1.0D0,1.0D0,1.0D0/
270 DATA M,KPLUS1,NROWS,NPLUS1/4,3,3,3/
271 DO 8 I = 1,3
```

```
272 DO 5 J = 1,13
273 K(J) = KCR(I,J)
274 5 C(J) = CCR(I,J)
275 CALL E02BBF(NCAP7,K,C,XARG,FIT,IFAIL)
276 8 Y(I+1) = FIT
277 CALL E02ADF(M,KPLUS1,NROWS,X,Y,W,WORK1,WORK2,A,S,IFAIL)
278 DO 12 I = 1,3
279 12 B(I) = A(3,I)
280 XCAP = (2.0D0*CONC-X(4))/X(4)
281 CALL E02AEF(NPLUS1,B,XCAP,DCR,IFAIL)
282 END
283 ************************************************************************
284 SUBROUTINE COBALT(CONC,XARG,DCO)
285 DOUBLE PRECISION K(13),KCO(3,13),C(13),CCO(3,13),FIT,XARG
286 DOUBLE PRECISION X(4),Y(4),W(4),WORK1(3,4),WORK2(2,3)
287 DOUBLE PRECISION A(3,3),S(3),B(3),CONC,DCO,XCAP
288 INTEGER M,KPLUS1,NROWS,IFAIL,NPLUS1
289 DATA CCO(1,1),CCO(1,2),CCO(1,3)/1.975D1,2.39D1,2.87D1/,
290 * CCO(1,4),CCO(1,5),CCO(1,6),CCO(1,7)/2.36D1,6.94D0,2.81D0,4.36D0/
291 * ,CCO(1,8),CCO(1,9),CCO(1,10)/1.89D0,1.47D0,0.0D0/,
292 * CCO(1,11),CCO(1,12),CCO(1,13)/0.0D0,0.0D0,0.0D0/,
293 * CCO(2,1),CCO(2,2),CCO(2,3),CCO(2,4)/1.58D1,7.87D0,2.36D0,1.78D0/
294 * ,CCO(2,5),CCO(2,6),CCO(2,7)/1.8D1,8.52D0,3.82D0/,
295 * CCO(2,8),CCO(2,9),CCO(2,10)/6.15D0,3.92D0,0.0D0/,
296 * CCO(2,11),CCO(2,12),CCO(2,13),CCO(3,1)/0.0D0,0.0D0,0.0D0,3.51D1/
297 * ,CCO(3,2),CCO(3,3),CCO(3,4)/4.08D1,3.59D1,4.98D1/,
298 * CCO(3,5),CCO(3,6),CCO(3,7)/-1.87D1,3.59D1,2.365D1/
299 DATA CCO(3,8),CCO(3,9),CCO(3,10)/1.88D1,1.09D1,0.0D0/,
300 * CCO(3,11),CCO(3,12),CCO(3,13),KCO(1,1)/0.0D0,0.0D0,0.0D0,1.0D2/,
301 * KCO(1,2),KCO(1,3),KCO(1,4),KCO(1,5)/1.0D2,1.0D2,1.0D2,1.4D2/,
302 * KCO(1,6),KCO(1,7),KCO(1,8),KCO(1,9)/2.0D2,3.1D2,4.2D2,6.0D2/,
303 * KCO(1,10),KCO(1,11),KCO(1,12)/7.5D2,7.5D2,7.5D2/,
304 * KCO(1,13),KCO(2,1),KCO(2,2),KCO(2,3)/7.5D2,1.0D2,1.0D2,1.0D2/,
305 * KCO(2,4),KCO(2,5),KCO(2,6),KCO(2,7)/1.0D2,1.5D2,1.7D2,2.4D2/,
306 * KCO(2,8),KCO(2,9),KCO(2,10)/3.286D2,4.25D2,7.5D2/,
307 * KCO(2,11),KCO(2,12),KCO(2,13),KCO(3,1)/7.5D2,7.5D2,7.5D2,1.0D2/,
308 * KCO(3,2),KCO(3,3),KCO(3,4),KCO(3,5)/1.0D2,1.0D2,1.0D2,1.3D2/,
309 * KCO(3,6),KCO(3,7),KCO(3,8),KCO(3,9)/1.6D2,2.1D2,2.5D2,3.4D2/,
310 * KCO(3,10),KCO(3,11),KCO(3,12),KCO(3,13)/7.5D2,7.5D2,7.5D2,7.5D2/
```

```
311 DATA NCAP7,IFAIL/13,0/
312 DATA X(1),X(2),X(3),X(4),Y(1)/0.0D0,1.44D0,2.83D0,5.56D0,0.0D0/,
313 * W(1),W(2),W(3),W(4)/1.0D3,1.0D0,1.0D0,1.0D0/
314 DATA M,KPLUS1,NROWS,NPLUS1/4,3,3,3/
315 DO 8 I = 1,3
316 DO 5 J = 1,13
317 K(J) = KCO(I,J)
318 5 C(J) = CCO(I,J)
319 CALL E02BBF(NCAP7,K,C,XARG,FIT,IFAIL)
320 8 Y(I+1) = FIT
321 CALL E02ADF(M,KPLUS1,NROWS,X,Y,W,WORK1,WORK2,A,S,IFAIL)
322 DO 12 I = 1,3
323 12 B(I) = A(3,I)
324 XCAP = (2.0D0*CONC-X(4))/X(4)
325 CALL E02AEF(NPLUS1,B,XCAP,DCO,IFAIL)
326 END
327 ************************************************************************
328 SUBROUTINE PHOS(X,P,I1)
329 C
330 C CALCULATES STRENGTHENING DUE TO PHOSPHORUS AT 23DEGC
331 C
332 DOUBLE PRECISION X,P
333 DATA DTAUDC/1.28D2/
334 P = DTAUDC*X
335 IF (X.GT.1.98D-1) I1 = 1
336 END
337 ************************************************************************
338 SUBROUTINE RESULT(DSRES,ELSE,I2,I555)
339 DOUBLE PRECISION C(15),DAT(15),DSRES(15),ELSE(15),TTLSUM(500)
340 DOUBLE PRECISION DSB,DSC,DSN,FE,SUM1,SUM2,SYFE,T,TOTAL
341 INTEGER I2(15)
342 COMMON/TOT/TTLSUM
343 COMMON/PARMS/C,DAT,T
344 C
345 C COMMON BLOCK SHC CONNECTS TO FINAL SUBROUTINE FOR
346 C CALCULATION OF STRAIN HARDENING COEFFICIENTS
347 C
348 COMMON/SHC/TOTAL
349 WRITE(6,20)T,T-273
```

```
350 CALL IRON(T,SYFE)
351 IF (DAT(13).GT.0.0D0) CALL CARBON(DSC)
352 DO 10 I = 1,12
353 IF (DAT(I).GT.0.0D0) THEN
354 CALL NAME(I)
355 WRITE(6,50)DAT(I),C(I)
356 IF (I.LE.5 .OR. I.EQ.12) WRITE(6,46)
357 IF (I.EQ.6) WRITE(6,47)
358 IF (I.EQ.8 .OR. I.EQ.9) WRITE(6,47)
359 IF (I2(I).EQ.1) WRITE(6,49)
360 IF (T.EQ.2.96D2) THEN
361 WRITE(6,60)2.0D0*DSRES(I)
362 IF (I.LE.5) WRITE(6,61)ELSE(I)
363 IF (I.EQ.2) WRITE(6,65)
364 ELSE
365 IF (I.LE.5) THEN
366 WRITE(6,51)
367 WRITE(6,60)ELSE(I)
368 ELSE
369 WRITE(6,52)
370 WRITE(6,60)2.0D0*DSRES(I)
371 ENDIF
372 ENDIF
373 ENDIF
374 10 CONTINUE
375 DSN = 0.0D0
376 DSB = 0.0D0
377 CALL NANDB(DSN,DSB)
378 SUM1 = SYFE + DSC + DSN + DSB - 2.0D0*DSRES(2) + ELSE(2)
379 SUM2 = SYFE + DSC + DSN + DSB
380 IF (T.EQ.2.96D2) TOTAL = 2.0D0*ADD(DSRES) + SUM1
381 IF (T.NE.2.96D2) TOTAL = ADD(ELSE) + SUM2
382 WRITE(6,70)TOTAL
383 TTLSUM(I555) = TOTAL
384 20 FORMAT(' AABS1.PROP:IRON',
385 * /,' FOR INFO SEE AABS1.PROP:SPEC',
386 * /,' FOR REFERENCES SEE AABS1.PROP:REFS',
387 * /,' ALL VALUES APPLY TO NORMAL YIELD STRESS',
388 * /,' TEMPERATURE =',F6.1,'K(',F5.1,'DEGC)'/)
```

```
   389 46 FORMAT(' STRAIN RATE = 0.25E-3/S')
   390 47 FORMAT(' STRAIN RATE IN RANGE 0.1E-4 TO 0.1E-2/S')
   391 49 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
   392 50 FORMAT(F7.4,' WT%(',F4.2,' AT%)')
   393 51 FORMAT(' TEMPERATURE DEPENDENT CALCULATION')
   394 52 FORMAT(' AS FOR 23DEGC')
   395 60 FORMAT(' DELTA SIGMA =',F6.2,'MPA')
   396 61 FORMAT(' (TEMPERATURE DEPENDENT CALCULATION: DELTA SIGMA
=',F6.2,
   397 *'MPA)')
   398 65 FORMAT(' ***TEMPERATURE DEPENDENT VALUE IS TAKEN***')
   399 70 FORMAT(/,' TOTAL =',F7.2,'MPA')
   400 END
   401 ************************************************************************
   402 SUBROUTINE IRON(T1,FE)
   403 C
   404 C ESTIMATES THE EFFECT OF TEMPERATURE AND STRAIN RATE ON THE
YIELD
   405 C STRESS OF PURE IRON USING DATA FROM CHRISTIAN AND ALTSHULER.
   406 C
   407 IMPLICIT DOUBLE PRECISION (F)
   408 DOUBLE PRECISION K(12),C(12),GRAD,REF,SRATE,T1,X1,X2,X3
   409 INTEGER NCAP7,IFAIL,I10
   410 COMMON/PARM/SRATE
   411 DATA C(1),C(2),C(3),C(4),C(5)/6.78D1,5.83D1,6.75D1,5.0D1,4.05D1/,
   412 * C(6),C(7),C(8),C(9),C(10)/2.66D1,2.4D1,2.25D1,0.0D0,0.0D0/,
   413 * C(11),C(12),K(1),K(2),K(3)/0.0D0,0.0D0,1.0D2,1.0D2,1.0D2/,
   414 * K(4),K(5),K(6),K(7),K(8)/1.0D2,1.4D2,1.9D2,2.25D2,2.6D2/,
   415 * K(9),K(10),K(11),K(12)/3.0D2,3.0D2,3.0D2,3.0D2/
   416 DATA FE296,FE300,REF/2.3D1,2.26D1,4.0D-4/
   417 DATA NCAP7,IFAIL,I10/12,0,0/
   418 IF (T1.GE.2.6D2) THEN
   419 SRATE=2.5D-4
   420 IF (SRATE.EQ.0.0D0) SRATE = 4.0D-4
   421 ELSE
   422 IF (T1.GT.1.65D2 .AND. T1.LE.1.95D2) THEN
   423 IF (SRATE.EQ.0.0D0) SRATE = 4.0D-4
   424 ELSE
   425 IF (SRATE.EQ.0.0D0) SRATE = 5.0D-4
```

```
426 REF = 5.0D-4
427 I10 = 1
428 ENDIF
429 ENDIF
430 GRAD = 2.38D0 + (1.84D-3*T1)
431 X1 = DLOG10(REF)
432 X2 = DLOG10(SRATE)
433 X3 = (X1-X2)*GRAD
434 IF (T1.GE.3.0D2) THEN
435 FE = (FE300 - X3)*9.80665D0
436 C
437 C THIS ASSUMPTION IS BASED ON FIG. 6 OF CONRAD AND FREDRICK, WHICH
438 C SHOWS THERE TO BE LITTLE CHANGE IN STRENGTH WITH TEMPERATURE ABOVE
439 C 300K. THEIR DATA IS NOT USED BECAUSE THEIR IRON WAS NOT VERY PURE.
440 C THE 9.80665 FACTOR CONVERTS KGF.MM-2 TO MPA.
441 C
442 WRITE(6,810)T1,FE,SRATE
443 IF (T1.GT.3.0D2) WRITE(6,825)
444 IF (T1.GT.3.0D2 .AND. SRATE.NE.4.0D-4) WRITE(6,830)
445 ELSE
446 CALL E02BBF(NCAP7,K,C,T1,FE,IFAIL)
447 FE = (FE - X3)*9.80665D0
448 WRITE(6,810)T1,FE,SRATE
449 IF (I10.EQ.1) WRITE(6,820)
450 IF (SRATE.GT.1.0D-2 .OR. SRATE.LT.3.2D-6) WRITE(6,840)
451 IF (SRATE.LT.3.0D-4 .AND. T1.GE.1.5D2) CALL KIMURA(T1,SRATE,X3)
452 FE296 = (FE296 - X3)
453 IF (T1.LT.2.96D2) WRITE(6,850) FE-FE296
454 ENDIF
455 810 FORMAT(' UPPER YIELD STRESS OF PURE IRON AT',F6.1,'K =',F7.2,'MPA'
456 *,
457 * /,' STRAIN RATE =',E9.2,'/S')
458 820 FORMAT(' BUT N.B., STRAIN RATE DATA IS ONLY APPROXIMATE AT THIS TE
459 *MPERATURE')
460 825 FORMAT(' ***TEMPERATURE SCALE EXTRAPOLATED***')
```

```
 830 FORMAT(' AN ATTEMPT HAS BEEN MADE TO ALLOW FOR STRAIN RATE')
 840 FORMAT(' ***STRAIN RATE EXTRAPOLATED***')
 850 FORMAT(' DIFFERENCE FROM SIGMA(296K) = +',F5.2,'MPA')
 END
 ************************************************************************
 SUBROUTINE KIMURA(T2,STRAT,X4)
 C
 C ESTIMATES THE EFFECT OF TEMPERATURE AND STRAIN RATE ON THE YIELD
 C STRESS OF PURE IRON, COMBINING DATA FROM KIMURA ET AL. WITH RESULTS
 C FROM CHRISTIAN AND ALTSHULER
 C
 DOUBLE PRECISION K(11),C(11),FE,T2,STRAT,X4
 INTEGER NCAP7,IFAIL
 DATA C(1),C(2),C(3),C(4),C(5)/2.0D2,1.95D2,1.78D2,8.92D1,6.21D1/,
 * C(6),C(7),C(8),C(9),C(10)/4.28D1,3.51D1,0.0D0,0.0D0,0.0D0/,
 * C(11),K(1),K(2),K(3),K(4)/0.0D0,1.5D2,1.5D2,1.5D2,1.5D2/,
 * K(5),K(6),K(7),K(8),K(9)/2.2D2,2.4D2,2.65D2,3.0D2,3.0D2/,
 * K(10),K(11)/3.0D2,3.0D2/
 DATA NCAP7,IFAIL/11,0/
 CALL E02BBF(NCAP7,K,C,T2,FE,IFAIL)
 FE = FE - X4
 WRITE(6,880)FE
 IF (SRATE.NE.8.3D-5) WRITE(6,890)
 880 FORMAT(' ALTHOUGH C.F.: SIGMA 0.1/LYS (REF. KIMURA ET AL.):',
 *F6.2,'MPA')
 890 FORMAT(' (STRAIN RATE EXTRAPOLATED FROM 8.3E-5/S)')
 END
 ************************************************************************
 SUBROUTINE CARBON(DC1SS)
 C
 C CALCULATES STRENGTHENING DUE TO CARBON AT ROOM T:
 C 29.4.87: STRENGTHENING DUE TO CARBON TAKEN AS ZERO
 C
 DOUBLE PRECISION C(15),DAT(15),DC1,DC1SS,DC2,DC3,T
 COMMON/PARMS/C,DAT,T
 CALL NAME(13)
 WRITE(6,910)DAT(13),C(13)
```

```
498 DC1SS = 0.0D0
499 IF (DAT(13).LE.5.0D-3) WRITE(6,920)
500 DC1 = C(13)/1.0D2
501 DC1 = (6.259D2*SQRT(DC1))*1.54443D1
502 C
503 C THE 1.54443D1 FACTOR CONVERTS TONS.IN-2 TO MPA
504 C
505 WRITE(6,940)DC1
506 C
507 C ALLOWS FOR THE LOW SOLUBILITY OF C IN FE
508 C
509 WRITE(6,945)DC1SS
510 IF (C(13).GT.9.694D-1) WRITE(6,950)
511 DC2 = C(13)/1.0D2
512 DC2 = (6.875D2*DSQRT(DC2))*1.54443D1
513 WRITE(6,960)DC2
514 IF (C(13).GT.1.235D0) WRITE(6,950)
515 DC3 = (3.802D1*DAT(13) + 2.551D1*DAT(13)*DAT(13))*6.89476D0
516 C
517 C THE 6.89476D0 FACTOR CONVERTS 1000PSI TO MPA
518 C
519 WRITE(6,980)DC3
520 910 FORMAT(F6.3,' WT%(',F4.2,' AT%)')
521 920 FORMAT(' NOTE: ACCURATE DATA ON THE STRENGTHENING DUE TO
CARBON AT
522 * THIS',/,' CONCENTRATION IS AVAILABLE, (REFS. BAIN AND PAXTON/KIMU
523 *RA ET AL.).')
524 940 FORMAT(' N.B. HIGH NICKEL (20-30WT%) STEEL DATA /0.2PS
COMPRESSION
525 *', /,' STRENGTHENING IS ESSENTIALLY ATHERMAL (REF. CHRISTIAN)',
526 * /,' LATH MARTENSITE: DELTA SIGMA =',F7.2,'MPA')
527 945 FORMAT(' => STRENGTHENING DUE TO CARBON IN SOLUTION: DELTA
SIGMA =
528 *',F6.2,'MPA')
529 950 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
530 960 FORMAT(' (TWINNED MARTENSITE: DELTA SIGMA =',F7.2,'MPA)')
531 980 FORMAT(' INFLUENCE OF CARBON ON YIELD STRENGTH OF STEEL
SECTIONS,'
532 *, /,' (REF. BAIN AND PAXTON):',F6.2,'MPA')
```

```
C
      DOUBLE PRECISION C(15),DAT(15),CB(9),KB(9)
      DOUBLE PRECISION BOR,DB,DBB,DN,NIT,NIT200,NIT300,PPM,T
      INTEGER NCAP7,IFAIL
      COMMON/PARMS/C,DAT,T
      DATA CB(1),CB(2),CB(3),CB(4)/0.0D0,1.0D2,1.21D2,1.21D2/,
     * CB(5),CB(6),CB(7),CB(8),CB(9)/1.24D2,0.0D0,0.0D0,0.0D0,0.0D0/
     * ,KB(1),KB(2),KB(3),KB(4)/0.0D0,0.0D0,0.0D0,0.0D0/,
     * KB(5),KB(6),KB(7),KB(8),KB(9)/2.5D1,1.4D2,1.4D2,1.4D2,1.4D2/
      DATA BOR,NIT/3.151D4,4.344D3/
      DATA NCAP7,IFAIL/9,0/
      DO 88 I = 14,15
      IF (C(I).GT.0.0D0) THEN
      CALL NAME(I)
      IF (I.EQ.14) THEN
      IF (DAT(14).EQ.0.0D0) THEN
      DN = 0.0D0
      ELSE
      NIT200 = 2.58 - (5.31D3*DAT(14)) + 1.455D5*DAT(14)*DAT(14)
      NIT300 = 7.35 + (0.44D4*DAT(14)) - 0.594D5*DAT(14)*DAT(14)
      DN = 1.0D-2*(NIT300-NIT200)*(T-2.0D2) + NIT200
      ENDIF
      WRITE(6,1010)DAT(14),C(14)*1.0D4,C(14),DN
      ELSE
      PPM = C(15)*1.0D4
      IF (PPM.LT.1.4D2) THEN
      CALL E02BBF(NCAP7,KB,CB,PPM,DB,IFAIL)
      WRITE(6,1015)DAT(15),PPM,C(15),DB
      ELSE
      WRITE(6,1020)
      ENDIF
      DBB = DAT(15)*BOR
      WRITE(6,1030)DBB
      ENDIF
      ENDIF
   88 CONTINUE
 1010 FORMAT(F7.4,' WT%(',F4.0,' ppm.atoms/',F6.4,' AT%)',
     * /,' DELTA SIGMA =',F6.2,'MPA',
     * /,' (APPROX.)')
```

```
498 DC1SS = 0.0D0
499 IF (DAT(13).LE.5.0D-3) WRITE(6,920)
500 DC1 = C(13)/1.0D2
501 DC1 = (6.259D2*SQRT(DC1))*1.54443D1
502 C
503 C THE 1.54443D1 FACTOR CONVERTS TONS.IN-2 TO MPA
504 C
505 WRITE(6,940)DC1
506 C
507 C ALLOWS FOR THE LOW SOLUBILITY OF C IN FE
508 C
509 WRITE(6,945)DC1SS
510 IF (C(13).GT.9.694D-1) WRITE(6,950)
511 DC2 = C(13)/1.0D2
512 DC2 = (6.875D2*DSQRT(DC2))*1.54443D1
513 WRITE(6,960)DC2
514 IF (C(13).GT.1.235D0) WRITE(6,950)
515 DC3 = (3.802D1*DAT(13) + 2.551D1*DAT(13)*DAT(13))*6.89476D0
516 C
517 C THE 6.89476D0 FACTOR CONVERTS 1000PSI TO MPA
518 C
519 WRITE(6,980)DC3
520 910 FORMAT(F6.3,' WT%(',F4.2,' AT%)')
521 920 FORMAT(' NOTE: ACCURATE DATA ON THE STRENGTHENING DUE TO
CARBON AT
522 * THIS',/,' CONCENTRATION IS AVAILABLE, (REFS. BAIN AND PAXTON/KIMU
523 *RA ET AL.).')
524 940 FORMAT(' N.B. HIGH NICKEL (20-30WT%) STEEL DATA /0.2PS
COMPRESSION
525 *', /,' STRENGTHENING IS ESSENTIALLY ATHERMAL (REF. CHRISTIAN)',
526 * /,' LATH MARTENSITE: DELTA SIGMA =',F7.2,'MPA')
527 945 FORMAT(' => STRENGTHENING DUE TO CARBON IN SOLUTION: DELTA
SIGMA =
528 *',F6.2,'MPA')
529 950 FORMAT(' ***CONCENTRATION EXTRAPOLATED***')
530 960 FORMAT(' (TWINNED MARTENSITE: DELTA SIGMA =',F7.2,'MPA)')
531 980 FORMAT(' INFLUENCE OF CARBON ON YIELD STRENGTH OF STEEL
SECTIONS,'
532 *, /,' (REF. BAIN AND PAXTON):',F6.2,'MPA')
```

```
533 END
534 ************************************************************************
535 SUBROUTINE NAME(M)
536 IF (M.EQ.1) WRITE(6,31)
537 IF (M.EQ.2) WRITE(6,32)
538 IF (M.EQ.3) WRITE(6,33)
539 IF (M.EQ.4) WRITE(6,34)
540 IF (M.EQ.5) WRITE(6,35)
541 IF (M.EQ.6) WRITE(6,36)
542 IF (M.EQ.7) WRITE(6,37)
543 IF (M.EQ.8) WRITE(6,38)
544 IF (M.EQ.9) WRITE(6,39)
545 IF (M.EQ.10) WRITE(6,40)
546 IF (M.EQ.11) WRITE(6,41)
547 IF (M.EQ.12) WRITE(6,42)
548 IF (M.EQ.13) WRITE(6,43)
549 IF (M.EQ.14) WRITE(6,44)
550 IF (M.EQ.15) WRITE(6,45)
551 31 FORMAT(/,' NICKEL')
552 32 FORMAT(/,' MANGANESE')
553 33 FORMAT(/,' SILICON')
554 34 FORMAT(/,' CHROMIUM')
555 35 FORMAT(/,' COBALT')
556 36 FORMAT(/,' VANADIUM')
557 37 FORMAT(/,' TITANIUM')
558 38 FORMAT(/,' MOLYBDENUM')
559 39 FORMAT(/,' ALUMINIUM')
560 40 FORMAT(/,' NIOBIUM')
561 41 FORMAT(/,' DUMMY')
562 42 FORMAT(/,' PHOSPHORUS')
563 43 FORMAT(/,' CARBON')
564 44 FORMAT(/,' NITROGEN')
565 45 FORMAT(/,' BORON')
566 END
567 ************************************************************************
568 SUBROUTINE NANDB(DN,DBB)
569 C
570 C CALCULATES STRENGTHENING DUE TO NITROGEN AND BORON AT ROOM
T
```

```
C
      DOUBLE PRECISION C(15),DAT(15),CB(9),KB(9)
      DOUBLE PRECISION BOR,DB,DBB,DN,NIT,NIT200,NIT300,PPM,T
      INTEGER NCAP7,IFAIL
      COMMON/PARMS/C,DAT,T
      DATA CB(1),CB(2),CB(3),CB(4)/0.0D0,1.0D2,1.21D2,1.21D2/,
     * CB(5),CB(6),CB(7),CB(8),CB(9)/1.24D2,0.0D0,0.0D0,0.0D0,0.0D0/
     * ,KB(1),KB(2),KB(3),KB(4)/0.0D0,0.0D0,0.0D0,0.0D0/,
     * KB(5),KB(6),KB(7),KB(8),KB(9)/2.5D1,1.4D2,1.4D2,1.4D2,1.4D2/
      DATA BOR,NIT/3.151D4,4.344D3/
      DATA NCAP7,IFAIL/9,0/
      DO 88 I = 14,15
      IF (C(I).GT.0.0D0) THEN
      CALL NAME(I)
      IF (I.EQ.14) THEN
      IF (DAT(14).EQ.0.0D0) THEN
      DN = 0.0D0
      ELSE
      NIT200 = 2.58 - (5.31D3*DAT(14)) + 1.455D5*DAT(14)*DAT(14)
      NIT300 = 7.35 + (0.44D4*DAT(14)) - 0.594D5*DAT(14)*DAT(14)
      DN = 1.0D-2*(NIT300-NIT200)*(T-2.0D2) + NIT200
      ENDIF
      WRITE(6,1010)DAT(14),C(14)*1.0D4,C(14),DN
      ELSE
      PPM = C(15)*1.0D4
      IF (PPM.LT.1.4D2) THEN
      CALL E02BBF(NCAP7,KB,CB,PPM,DB,IFAIL)
      WRITE(6,1015)DAT(15),PPM,C(15),DB
      ELSE
      WRITE(6,1020)
      ENDIF
      DBB = DAT(15)*BOR
      WRITE(6,1030)DBB
      ENDIF
      ENDIF
   88 CONTINUE
 1010 FORMAT(F7.4,' WT%(',F4.0,' ppm.atoms/',F6.4,' AT%)',
     * /,' DELTA SIGMA =',F6.2,'MPA',
     * /,' (APPROX.)')
```

```
610 1015 FORMAT(F7.4,' WT%(',F4.0,' ppm/',F6.4,' AT%)',
611 * /,' DERIVED FROM STEEL DATA /STRAIN RATE NOT GIVEN',
612 * /,' ROOM TEMPERATURE',
613 * /,' DELTA SIGMA =',F6.2,'MPA')
614 1020 FORMAT(' ***MAX. CONCENTRATION IS 0.0027WT%(140PPM), BUT...')
615 1030 FORMAT(' C.F.: 0.2PS (REF. IRVINE AND PICKERING):',F7.2,'MPA')
616 END
617 ************************************************************************
618 SUBROUTINE NCALC (YLDSTR, VAL, VAC)
619 IMPLICIT REAL*8 (A-H,O-$)
620 COMMON/SHC/SUM
621 DATA ENM/1.0D-4/
622 VAL = VAL/1.0D2
623 VAC = VAC/1.0D2
624 VW = 1.0 - VAL - VAC
625 SY = VAL*124.4D0*((0.002D0)**0.644D0)
626 SY = SY + VW*478.1D0*((0.002D0)**0.0812D0)
627 SY = SY + VAC*498.5D0*((0.002D0)**0.103D0)
628 SUTS = VAL*124.4D0*((0.644D0)**0.644D0)
629 SUTS = SUTS + VW*478.1D0*((0.0812D0)**0.0812D0)
630 SUTS = SUTS + VAC*498.5D0*((0.103D0)**0.103D0)
631 C
632 C ITERATION TO FIND STRAIN HARDENING COEFFICIENT
633 C
634 SY = SY + SUM
635 SUTS = SUTS + SUM
636 4 CONTINUE
637 ARGUM = (SY/SUTS) - ((0.002D0/ENM)**ENM)
638 ENM = ENM + 1.D-6
639 IF (ARGUM.LT.0.00001D0) GOTO 4
640 YLDSTR = YLDSTR*(0.1D0**ENM)
641 RETURN
642 END
643 %
644 FILE .DATA TO .OUT:ONE
645 FILE .OUT:TWO TO &A
646 COMMENT DATA IS IN .OUT:ONE
647 COMMENT RESULTS ARE IN .OUT:TWO
648 COMMENT COPY FOR EDITING IS IN &A
```

APPENDIX 5: STRAIN-HARDENING COEFFICIENTS PROGRAM

```
1 FTVSCLR PROGRAM=%H% DATA=.NREG:DATA NAG OUTPUT=&OUT
2 C COPYRIGHT A. A. B. SUGDEN 1988.
3 C MINIMIZATION PROGRAM FOR EVALUATION OF STRAIN-HARDENING COEFFICIENTS
4 C KEY: X(3) = KAL = K alpha
5 C X(2) = KW = K W
6 C X(1) = KAC = K a
7 C X(4) = NAL = n alpha
8 C X(5) = NW = n W
9 C X(6) = NAC = n a
10 C
11 IMPLICIT REAL*8(A-H,K,N-$)
12 DOUBLE PRECISION SIGMY(35), SIGUTS(35), VAL(35), VW(35), VAC(35)
13 DOUBLE PRECISION FVEC(6), WA(100), X(6)
14 DOUBLE PRECISION DIAG(8), FJAC(7,7), R(30), QTF(6), W(6,5)
15 COMMON/AABS1/SIGMY,SIGUTS,VAL,VW,VAC
16 EXTERNAL FCN
17 DATA MAXFEV, ML, MU, MODE, MPRINT/ 1500, 5, 5, 1, 1/
18 DATA XTOL, EPSFCN, FACTOR / 1.0D-7, 0.0D0, 100.0D0/
19 DATA LDFJAC, LR, IFAIL/ 7, 30, 0/
20
21 DO 4 I = 1,35
22 READ(5,*)SIGMY(I), SIGUTS(I), VAL(I), VAC(I)
23 4 VW(I) = 1.0D0 - VAL(I) - VAC(I)
24 CALL C05NCF(FCN,6,X,FVEC,XTOL,MAXFEV,ML,MU,
25 1 EPSFCN,DIAG,MODE,FACTOR,MPRINT,MFEV,FJAC,LDFJAC,
26 2 R,LR,QTF,W,IFAIL)
27 FNORM=F05ABF(FVEC,6)
28 33 WRITE(6,55)X(3),X(2),X(1),X(4),X(5),X(6)
29 STOP
30 55 FORMAT(' KAL =',F11.6,/,' KW =',F11.6,/,
31 &' KAC =',F11.6,/,' NAL =',F9.6,/,
32 &' NW =',F9.6,/,' NAC =',F9.6)
33 END
34
35 SUBROUTINE FCN(J,X,EQN,IFLAG)
36 IMPLICIT REAL*8(A-H,K,N-$)
37 DOUBLE PRECISION SIGMY(35), SIGUTS(35), VAL(35), VW(35), VAC(35)
```

```
38 DOUBLE PRECISION EQN(6),X(6)
39 COMMON/AABS1/SIGMY,SIGUTS,VAL,VW,VAC
40 J = 6
41 IF (J1.EQ.0) THEN
42 C
43 C INITIAL GUESS VALUES
44 C
45 X(3) = 202.0D0
46 X(2) = 504.0D0
47 X(1) = 526.0D0
48 X(4) = 0.595D0
49 X(5) = 0.072D0
50 X(6) = 0.094D0
51 ENDIF
52 J1 = 1
53 WRITE(6,77)X(3),X(2),X(1),X(4),X(5),X(6)
54 SUMMY = ADD(SIGMY)
55 SUMVAL = ADD(VAL)
56 SUMVW = ADD(VW)
57 SUMVAC = ADD(VAC)
58 SUMUTS = ADD(SIGUTS)
59 ARGY = SUMMY - SUMVAL*X(3)*((0.002D0)**X(4))
60 ARGY = ARGY - SUMVW*X(2)*((0.002D0)**X(5))
61 ARGY = ARGY - SUMVAC*X(1)*((0.002D0)**X(6))
62 ARGUTS = SUMUTS - SUMVAL*X(3)*(X(4)**X(4))
63 ARGUTS = ARGUTS - SUMVW*X(2)*(X(5)**X(5))
64 ARGUTS = ARGUTS - SUMVAC*X(1)*(X(6)**X(6))
65 EQN(1) = ARGY*SUMVAL*((0.002D0)**X(4))
66 EQN(1) = EQN(1) + ARGUTS*SUMVAL*(X(4)**X(4))
67 EQN(2) = ARGY*SUMVW*((0.002D0)**X(5))
68 EQN(2) = EQN(2) + ARGUTS*SUMVW*(X(5)**X(5))
69 EQN(3) = ARGY*SUMVAC*((0.002D0)**X(6))
70 EQN(3) = EQN(3) + ARGUTS*SUMVAC*(X(6)**X(6))
71 EQN(4) = ARGY*SUMVAL*X(3)*(-6.2146D0)*((0.002D0)**X(4))
72 E4 = ARGUTS*SUMVAL*X(3)*(X(4)**X(4))*(1.0D0+DLOG(X(4)))
73 EQN(4) = EQN(4) + E4
74 EQN(5) = ARGY*SUMVW*X(2)*(-6.2146D0)*((0.002D0)**X(5))
75 EQN5 = ARGUTS*SUMVW*X(2)*(X(5)**X(5))*(1.0D0+DLOG(X(5)))
76 EQN(5) = EQN(5) + E5
```

```
77 EQN(6) = ARGY*SUMVAC*X(1)*(-6.2146D0)*((0.002D0)**X(6))
78 EQN6 = ARGUTS*SUMVAC*X(1)*(X(6)**X(6))*(1.0D0+DLOG(X(6)))
79 EQN(6) = EQN(6) + E6
80 WRITE(6,88) EQN(1),EQN(2),EQN(3),EQN(4),EQN(5),EQN(6)
81 RETURN
82 77 FORMAT(' KAL =',F11.6,/,' KW =',F11.6,/,
83 &' KAC =',F11.6,/,' NAL =',F9.6,/,
84 &' NW =',F9.6,/,' NAC =',F9.6)
85 88 FORMAT(' EQN1 =',E12.5,/,' EQN2 =',E12.5,/,
86 &' EQN3 =',E12.5,/,' EQN4 =',E12.5,/,
87 &' EQN5 =',E12.5,/,' EQN6 =',E12.5)
88 END
89
90 DOUBLE PRECISION FUNCTION ADD(Y)
91 DOUBLE PRECISION Y(35)
92 ADD = 0.0D0
93 DO 4 I = 1,35
94 4 ADD = ADD + Y(I)
95 RETURN
96 END
97 %
```

APPENDIX 6: HETEROGENEITY PROGRAM

```
1 FTVSCLR PROGRAM=%H% DATA=.DATA OUTPUT=&A
2 C CONCURRENT PROGRAM TO CALCULATE SCATTER AND HETEROGENEITY
3 C OF WELD METALS (TREATED AS A THREE PHASE MICROSTRUCTURE)
4 C COPYRIGHT A. A. B. SUGDEN, 1988.
5 READ(5,*)N,A,B
6 C READ NO. OF SETS OF DATA, AND
7 C VOLUME FRACTIONS OF TWO OF THE PHASES
8 WRITE(6,5)N
9 DO 4 I = 1,N
10 READ(5,*)T,E
11 C READ TESTING TEMPERATURES (IN DEGREES CELSIUS)
12 C AND CHARPY ENERGIES (IN JOULES)
13 4 WRITE(6,10)T,E
14 C OUTPUT IS IN A FORMAT SUITABLE FOR GLIM
15 C (GENERALISED LINEAR INTERACTIVE MODELLING PACKAGE)
16 WRITE(6,15)
17 STOP
18 5 FORMAT(' $ units',I3,' $ data temp e $ read')
19 10 FORMAT(2F8.2)
20 15 FORMAT(' $ ',/,
21 &' $ plot e temp $ ',/,
22 &' $ calc y=%log(e/(280-e)) $ plot y temp $ ',/,
23 C THE NUMBER 280 IS THE UPPER SHELF ENERGY
24 C AND SHOULD BE ALTERED ACCORDINGLY
25 &' $ yvar y $ fit $ dis e $ ',/,
26 &' $ fit + temp $ dis e r $ plot %fv temp $ ',/,
27 &' $ end',/,
28 &' $ stop')
29 END
30 %
31 !
32 GLIM PROGRAM=&A OUTPUT=&B
33 ! THIS PROGRAM CALCULATES THE MICROSTRUCTURAL
34 ! HETEROGENEITY OF THE THREE PHASE MICROSTRUCTURE
35 FTVSCLR %H% DATA=.DATA OUTPUT=&C
36 DOUBLE PRECISION B,C,D,HOMOG
37 READ(5,*)I,B,C
38 B = B/1.0D2
```

```
39 C = C/1.0D2
40 D = 1.0D0 - B - C
41 WRITE(6,45)B,C,D
42 HOMOG = 1.0D0 - B - C
43 HOMOG = HOMOG*(DLOG(HOMOG))
44 HOMOG = HOMOG + B*(DLOG(B))
45 HOMOG = HOMOG + C*(DLOG(C))
46 HOMOG = - HOMOG
47 WRITE(6,55)HOMOG
48 STOP
49 45 FORMAT(' VOLUME FRACTIONS :',F8.4,' :',F8.4,' :',F8.4)
50 55 FORMAT(' HETEROGENEITY =',F11.4,/,
51 &' WHERE 0 = HOMOGENEOUS',/,
52 &' AND 1.0986 = HETEROGENEOUS')
53 END
54 %
```

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