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More Complete Theory for the Calculation of the Martensite–Start Temperature in Steels

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(Received on September 8, 2011; accepted on September 30, 2011)

KEY WORDS: martensite; start temperature; stress induced; strain induced; size effect.

1. Introduction

The vital breakthrough in accounting for the influence of chemical composition on the martensite–start temperature (M_S) came some 50 years ago^{1–4)} when it was identified that the free energy change $\Delta G^{\gamma\alpha} = G_\alpha - G_\gamma$ for the transformation of austenite to martensite must reach a critical value $\Delta G_{M_S}^{\gamma\alpha}$ at the martensite–start temperature (M_S). Subsequent refinements included, for example, accounting for the Zener ordering of carbon atoms⁵⁾ and solid solution strengthening in rich alloys of iron^{6,7)} but the basic principle remains the same as in the pioneering work, based on $\Delta G_{M_S}^{\gamma\alpha}$.

The ability to calculate M_S has acquired renewed importance in the context of a large variety of steels, both commercial and experimental, which rely on transformation–induced plasticity, or which deal with ultra–fine austenite.^{8–11)} In the latter case, the localised islands or films of austenite are stabilised to martensitic transformation due to their small scale, or when parent austenite is created in a highly refined state by processes such as severe plastic deformation. Although the influence of applied stress in the elastic regime has been established since the days of Patel and Cohen in terms of a mechanical driving force which supplements the chemical term,¹²⁾ many modern experiments are concerned with the transformation of austenite during straining well beyond its yield strength.^{13,14)} This has caused considerable confusion in the literature since both stress and plastic strain are applied simultaneously, but most refer to this simply as “strain–induced transformation”. Tamura and co–workers¹⁵⁾ pointed out that many of the observations could be explained on the basis of stress alone, even when the deformation is plastic. Several recent studies support this contention, that so–called strain–induced martensite in studies where stress and strain have been applied simultaneously, can be explained on the basis of stress alone.^{16–21)}

Indeed, transformation textures for displacive products can often be explained on the basis of variant selection due to stress alone.²²⁾ There have been limited experiments in which the effect of strain alone was studied. In an elegant

study²³⁾ of pre–deformed single crystals of austenite, transformed on cooling to martensite, where variant selection occurred due to the anisotropic nature of the dislocation debris. However, such anisotropy should be reduced in polycrystalline samples where multiple slip should operate,²⁴⁾ and experiments on bainite growing in pre–strained austenite failed to reveal variant selection.

However, there are two special effects of large plastic strains that cannot be neglected. The scale of the austenite grain structure defined in terms of a mean lineal intercept is changed by the deformation. Secondly, the introduction of dislocation debris can mechanically stabilise the austenite.^{8,25–30)} Mechanical stabilisation occurs because the movement of glissile martensite–austenite interfaces is hindered by the dislocation debris, and can lead to a complete cessation of transformation. The phenomenon has recently been quantitatively expressed.³¹⁾

The aim of the present work was to create a model for the martensite–start temperature which takes all of the effects described above into account. It is emphasised that the individual and validated components of such a model already exist in the literature; the present work represents a hopefully useful consolidation of theory.

2. Method

The role of alloying elements and the Zener ordering of carbon atoms has already been dealt with previously by identifying the temperature at which the chemical free energy equals the critical value $\Delta G^{\gamma\alpha} = \Delta G_{M_S}^{\gamma\alpha}$ ^{5,32)} and the associated computer program and documentation are freely available.³³⁾

The influence of stress *per se* is expressed via a mechanical driving force¹²⁾ which supplements the chemical component, and has been estimated on the basis of the shape deformation of martensite as:³⁴⁾

$$\Delta G_{MECH} = -0.86\sigma \text{ for uniaxial tension}$$

$$\Delta G_{MECH} = -0.58\sigma \text{ for uniaxial compression} \dots (1)$$

where the driving force is in J mol^{-1} and the stress in MPa. Such calculations can in fact be done for arbitrary stress tensors,³⁵⁾ but most experiments are done in uniaxial mode.

It has been shown recently³⁶⁾ that the observed variations in M_S due to austenite grain size can be explained quantitatively in terms of the ability to detect the onset of transformation as martensite plates get finer in accordance with smaller austenite grains, resulting in the relationship:

$$M_S^0 - M_S = \frac{1}{b} \ln \left[\frac{1}{\bar{L}_\gamma^3} \left\{ \exp \left(-\frac{\ln(1-f)}{m} \right) - 1 \right\} + 1 \right] \dots (2)$$

where $b = 0.2689$, \bar{L}_γ in mm, is the mean lineal intercept, $m = 0.05$ is the aspect ratio of martensite plates, and M_S is defined when a fraction $f = 0.01$ of martensite is obtained. Note that the original model for calculating M_S ^{5,32)} was validated on a large dataset due to Steven and Haynes,³⁷⁾ where according to a related atlas of TTT diagrams,³⁸⁾ the austenite grain size is in the range ASTM number 2–6 ($\bar{L}_\gamma \approx 40 - 160 \mu\text{m}$). In this range, M_S is not sensitive to \bar{L}_γ which was therefore assumed to be $40 \mu\text{m}$ in order to calculate M_S^0 .

One effect of plastic strain prior to transformation is to alter \bar{L}_γ through a change in the shape of the austenite grains. This problem has been dealt with^{39,40)} for a large variety of deformations in which an equiaxed grain is strained, but for uniaxial tension or compression, the result is:

$$\frac{\bar{L}_0}{\bar{L}} = \frac{(1+3\sqrt{3})S_{11}^{0.5} + 3(S_{11}^3 + 2)^{0.5} S_{11}^{-1} + (2+2S_{11}^3)^{0.5} S_{11}^{-1}}{3(2\sqrt{3}+1)} \dots (3)$$

where $S_{11} = \exp\{\pm\varepsilon\}$ where $+\varepsilon$ and $-\varepsilon$ are the plastic strains in tension and compression respectively, and \bar{L}_0 and \bar{L} are the lineal intercepts in the undeformed and deformed states respectively.

The second effect of plastic strain through mechanical stabilisation is considered by calculating the additional driving force needed in order for the interface to overcome the dislocation density (ρ) created by strain prior to transformation.^{31,41)}

$$\Delta G_{STA} = \frac{\mu b}{8\pi(1-\nu)}(\rho^{0.5} - \rho_0^{0.5}) \text{ J m}^{-3}$$

with $\rho = 2 \times 10^{13} + 2 \times 10^{14} \varepsilon \text{ m}^{-2}$ (4)

where μ is the shear modulus of austenite at 80 GPa, $b = 0.252 \text{ nm}$ is the magnitude of the Burgers vector of the dislocations, and the Poisson's ratio $\nu = 0.27$. To summarise, the martensite-start temperature independent of grain size effect is obtained from

$$\Delta G^{\gamma\alpha} + \Delta G_{MECH} < \Delta G_{M_s}^{\gamma\alpha} - \Delta G_{STA} \dots\dots\dots (5)$$

and this result is then corrected for a grain size effect using Eq. (2). Some indicative calculations are illustrated in **Fig. 1**. The computer program capable of the calculations presented here can be downloaded freely from <http://www.msm.cam.ac.uk/map/steel/programs/mucg46B.htm>

We have assumed, with some justification,¹⁵⁻²¹⁾ that all of

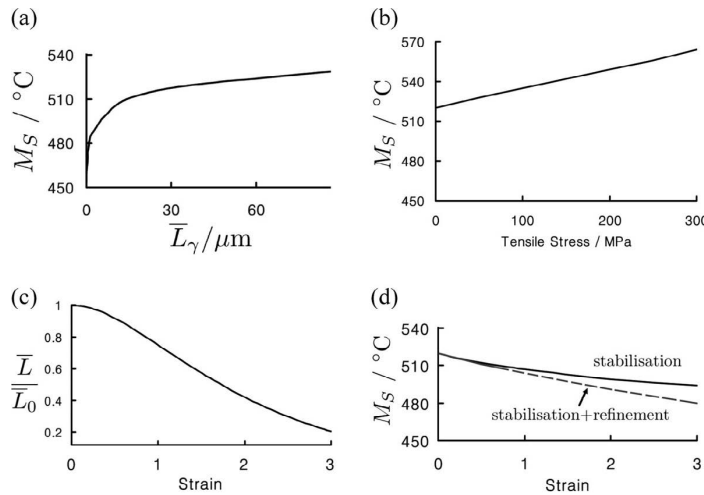


Fig. 1. Calculations for Fe-0.1C wt% steel. (a) Influence of austenite grain size. (b) Influence of tensile stress. (c) Change in mean linear intercept for austenite grains as a function of plastic strain. (d) The effect of mechanical stabilisation and grain refinement on the martensite start temperature.

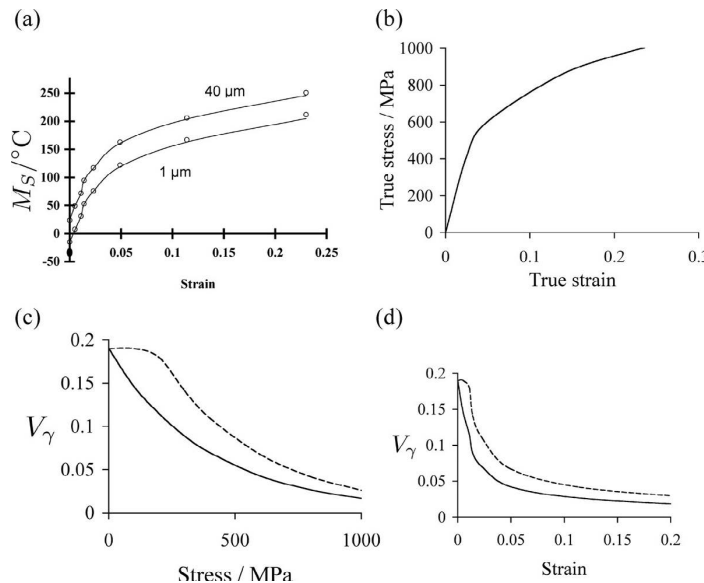


Fig. 2. (a) Plot of M_s as a function of the stress alone (points), or stress combined with both strain-effects (curves); (b) the stress-strain curve⁴³⁾ used to relate stress and strain. (c,d) V_γ as a function of stress or strain; the continuous and dashed lines represent \bar{L}_0 equal to 40 and 1 μm respectively.

the changes in M_S during uniaxial deformation can be explained solely in terms of stress, stabilisation and austenite grain refinement. In the theory of strain-induced martensite⁴²⁾ plastic strain influences the progress of transformation by introducing nucleation sites, but as pointed out, this does not seem to represent a large effect. Furthermore there are fitting parameters involved which have not been shown to be generally applicable. For this reason, we have not been able to include strain-induced nucleation into our model and remains a task for future work. The well-known nucleation of martensite at slip-bands and twin intersections naturally cannot be neglected so it is premature to conclude that strain-induced effects are always small. But it remains the case that when stress and strain are implemented simultaneously,^{15–21)} the observations can be rationalised largely on the basis of the mechanical driving force.

The calculations were applied to a typical TRIP-assisted steel of composition 0.23C–1.37Si–1.54Mn wt% containing a volume fraction $V_\gamma = 0.19$ of retained austenite,⁴³⁾ assumed to contain 1 wt% of carbon on average. The volume fractions were estimated using the calculated M_S temperatures and the Koistinen and Marburger equation.⁴⁴⁾ It is evident from Fig. 2(a) that for strains typical of TRIP-assisted steels, there is no substantial effect of plastic strain on the development of martensitic transformation, and stress alone can explain the TRIP phenomenon. Notice from Fig. 2(b) that the small austenite grain size has a substantial effect on the stability of the retained austenite, as is well known in the literature.

Acknowledgments

The authors are grateful for support from the POSCO Steel Innovation Programme, and to the World Class University Programme of the National Research Foundation of Korea, Ministry of Education, Science and Technology, project number R32–2008–000–10147–0.

REFERENCES

- 1) L. Kaufman and M. Cohen: *Prog. Met. Phys.*, **7** (1958), 165.
- 2) L. Kaufman, S. V. Radcliffe and M. Cohen: Thermodynamics of the bainite transformation, in *Decomposition of Austenite by Diffusional Processes*, ed. by V. F. Zackay and H. I. Aaronson, Interscience, New York, USA, (1962), 313.
- 3) Y. Imai, M. Izumiyama and M. Tsuchiya: *Sci. Rep. Res. Inst. Tohoku Univ.*, **A17** (1965), 173.
- 4) T. Bell and W. S. Owen: *Trans. Metall. Soc. AIME*, **239** (1967), 1940.
- 5) H. K. D. H. Bhadeshia: *Met. Sci.*, **15** (1981), 178.
- 6) G. Ghosh and G. B. Olson: *Acta Metall. Mater.*, **42** (1994), 3361.
- 7) G. Ghosh and G. B. Olson: *J. Phase Equilibria*, **22** (2001), 199.
- 8) W. C. Leslie and R. L. Miller: *ASM Trans. Quart.*, **57** (1964), 972.
- 9) H. Kitahara, N. Tsuji and Y. Minamino: *Mater. Sci. Eng. A*, **438–440** (2006), 233.
- 10) D. W. Suh, S. J. Park, T. H. Lee, C. S. Oh and S. J. Kim: *Metall. Mater. Trans. A*, **41** (2010), 397.
- 11) J. H. Ryu, D. I. Kim, H. S. Kim, H. K. D. H. Bhadeshia and D. W. Suh: *Scr. Mater.*, **63** (2010), 297.
- 12) J. R. Patel and M. Cohen: *Acta Metall.*, **1** (1953), 531.
- 13) K. Sugimoto, T. Sakaki, T. Kurihashi and O. Miyagawa: *Tetsu-to-Hagané*, **72** (1986), 2101.
- 14) M. Sherif, C. Garcia-Mateo, T. Sourmail and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **20** (2004), 319.
- 15) I. Tamura: *Met. Sci.*, **16** (1982), 245.
- 16) S. Chatterjee and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **23** (2007), 1101.
- 17) E. S. Perdahciouglu, H. J. M. Geijselaers and M. Groen: *Scr. Mater.*, **58** (2008), 947.
- 18) E. S. Perdahciouglu, H. J. M. Geijselaers and M. Groen: *Mater. Sci. Eng. A*, **481–482** (2008), 727.
- 19) S. Kundu and H. K. D. H. Bhadeshia: *Scr. Mater.*, **55** (2006), 779.
- 20) H. J. M. Geijselaers and E. S. Perdahciouglu: *Scr. Mater.*, **60** (2009), 29.
- 21) A. Das, P. C. Chakraborti, S. Tarafder and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **27** (2011), 366.
- 22) H. K. D. H. Bhadeshia: *ISIJ Int.*, **50** (2010), 1517.
- 23) J. C. Bokros and E. R. Parker: *Acta Metall.*, **11** (1963), 1291.
- 24) A. A. Shirzadi, H. Abreu, L. Pocock, D. Klobcar, P. J. Withers and H. K. D. H. Bhadeshia: *Int. J. Mater. Res.*, **100** (2009), 40.
- 25) E. S. Machlin and M. Cohen: *Trans. Metall. Soc. AIME*, **191** (1951), 746.
- 26) H. C. Fiedler, B. L. Averbach and M. Cohen: *Trans. Am. Soc. Met.*, **47** (1955), 267.
- 27) J. R. Strife, M. J. Carr and G. S. Ansell: *Metall. Trans. A*, **8A** (1977), 1471.
- 28) V. Raghavan: Kinetics of martensitic transformations, in *Martensite*, ed. by G. B. Olson and W. S. Owen, ASM International, Ohio, USA, (1992), 197.
- 29) K. Tsuzaki, S. Fukasaku, Y. Tomota and T. Maki: *Trans. JIM*, **32** (1991), 222.
- 30) H. K. D. H. Bhadeshia: *Mater. Sci. Eng. A*, **273–275** (1999), 58.
- 31) S. Chatterjee, H. S. Wang, J. R. Yang and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **22** (2006), 641.
- 32) H. K. D. H. Bhadeshia: *Met. Sci.*, **15** (1981), 175.
- 33) H. K. D. H. Bhadeshia: Software for transformations in steels, <http://www.msm.cam.ac.uk/map/steel/programs/mucg46-b.html>, (1982).
- 34) G. B. Olson and M. Cohen: *Metall. Trans. A*, **13** (1982), 1907.
- 35) S. Kundu, K. Hase and H. K. D. H. Bhadeshia: *P. Roy. Soc. A*, **463** (2007), 2309.
- 36) H. S. Yang and H. K. D. H. Bhadeshia: *Scr. Mater.*, **60** (2009), 493.
- 37) W. Steven and A. G. Haynes: *J. Iron Steel Inst.*, **183** (1956), 349.
- 38) Anonymous, Atlas of isothermal transformation diagrams, Special Report No. 56, The Iron and Steel Institute, London, UK, (1956).
- 39) S. B. Singh and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **15** (1998), 832.
- 40) J. Y. Chae, R. S. Qin and H. K. D. H. Bhadeshia: *ISIJ Int.*, **49** (2009), 115.
- 41) M. Maalekian, E. Kozeschnik, S. Chatterjee and H. K. D. H. Bhadeshia: *Mater. Sci. Technol.*, **23** (2007), 610.
- 42) G. B. Olson and M. Cohen: *Metall. Trans. A*, **6A** (1975), 791.
- 43) Z. Ki, D. Wu and R. Hu: *J. Iron Steel Res. Int.*, **13** (2006), 41.
- 44) D. P. Koistinen and R. E. Marburger: *Acta Metall.*, **7** (1959), 59.