Short Communication

Topology of grain deformation

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The deformation of a polycrystalline material leads to changes in the amount of grain surface and grain edge per unit volume. These parameters are of importance in kinetic theory since both surfaces and edges are heterogeneous nucleation sites. In the present study a method is described for calculating changes in the surface area and edge per unit volume as a function of common deformations encountered in the production of steels. Unlike previous analyses, each grain in the undeformed material is represented by a tetrakaidecahedron, a shape which is a realistic representation of equiaxed grains. There are some interesting results which are compared with previous work. MST/3898

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Introduction

The hot deformation of steel in its austenitic condition is the most common way of processing large quantities of material into their final shape. The deformation has the dual purpose of producing the required shape and refining the microstructure. During hot deformation, the austenite undergoes repeated recrystallisation, which leads to an increasingly smaller grain size. In the final stage of processing, the austenite is frequently left in a deformed state with a 'pancaked' grain structure since this enhances the possibility of obtaining a very fine ferrite grain structure.[1] The production process described here has many variants, including controlled rolling, thermomechanical controlled processing, etc. but they all involve the transformation of deformed austenite.

The development and manufacture of steel by controlled rolling is a very complicated process. There is, therefore, considerable research throughout the world to produce kinetic models dealing with the transformation of deformed austenite,[1–7] as an aid to the design of steels. Homogeneous deformation leads to an increase in the grain surface and grain edge per unit volume but there is no change in the number of grain corners per unit volume. Since surfaces, edges, and corners are all heterogeneous nucleation sites, any change in their number density must be taken into account in the kinetic model.

Umemoto *et al.*[2] estimated the change in the surface area of austenite grain surface per unit volume by representing the grains as spheres, each of unit radius. Rolling deformation changes the sphere into an ellipsoid with axes 1, $(1-p)$, and $1/(1-p)$, where p is the rolling reduction given by the change in thickness divided by the initial thickness. The surface area of the ellipsoidal grain is given by

$$A=\int_{-1/1-p}^{1/1-p}\left(\left\{4x\int_{0}^{\pi/2}[1-(2p-p^2)\sin^2\theta]^{1/2}d\theta\right\}\times\left[\frac{x^2(1-p)^6}{1-x^2(1-p)^2}+1\right]^{1/2}\right)dx \qquad (1)$$

which can be compared with the surface area of the original sphere as 4π. The method is a useful approximation but spheres are not space filling and do not have edges. We present here some calculations for the changes in surface and edge densities as a function of strain for grains which are initially in the form of Kelvin's space filling tetrakaidecahedra. This is probably the most realistic simple shape for equiaxed grains.[8]

Method

The deformation of a shape as complicated as a tetrakaidecahedron can be considered by representing each corner with a vector whose origin is conveniently chosen. The deformation itself can be described by a 3×3 deformation matrix,[9] which operates on each vector in turn to generate a set of new vectors defining the new shape. Thus, a vector $\boldsymbol{u}$ becomes a new vector $\boldsymbol{v}$ as a consequence of a homogeneous deformation $\mathbf{S}$

$$v=\mathbf{S}\boldsymbol{u}=\begin{pmatrix}b&0&0\\0&d&0\\0&0&c\end{pmatrix}\begin{pmatrix}u_1\\u_2\\u_3\end{pmatrix} \qquad (2)$$

where u_i are the components of $\boldsymbol{u}$, and b, d, and c are the principal distortions (ratios of the final to initial lengths of unit vectors along the principal axes). Therefore, $\ln(b)$, $\ln(d)$, and $\ln(c)$ are the true strains along the three principal axes of the deformation. Since all practical deformations involve shears only, there is no change in volume so that the determinant of $\mathbf{S}$ must be unity. It follows that $bcd=1$. Rolling involves plane strain deformation with $d=1$ and $bc=1$.

Results

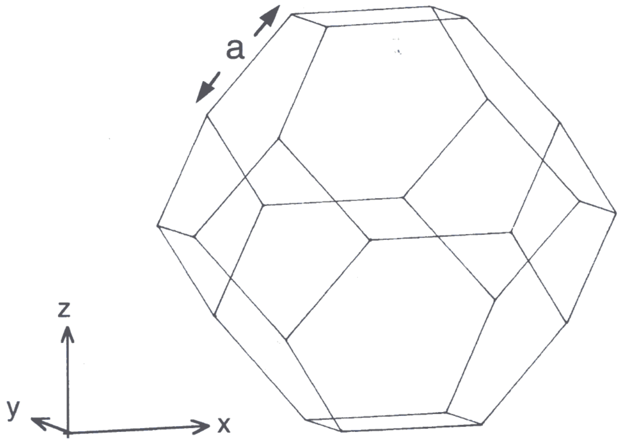
A tetrakaidecahedron has 14 faces consisting of 8 hexagons and 6 squares (Fig. 1). The resulting 36 edges each have a length a. The edges can be represented by just six non-parallel vectors whose components with respect to an origin defined at a corner are listed in Table 1, both before and after the deformation described by equation (2).

The surface area and edge length can easily be calculated using the vectors given in Table 1. Bearing in mind that $d=1/bc$ in order to retain a constant volume, the ratio A/A_0 of the surface area of the deformed to the undeformed tetrakaidecahedron is given by

$$\frac{A}{A_0}=\frac{b+3[b(1+2b^2c^4)^{1/2}+(b^2+2c^2)^{1/2}]+c[2(1+b^4c^2)]^{1/2}}{3bc(2\sqrt{3}+1)} \qquad (3)$$

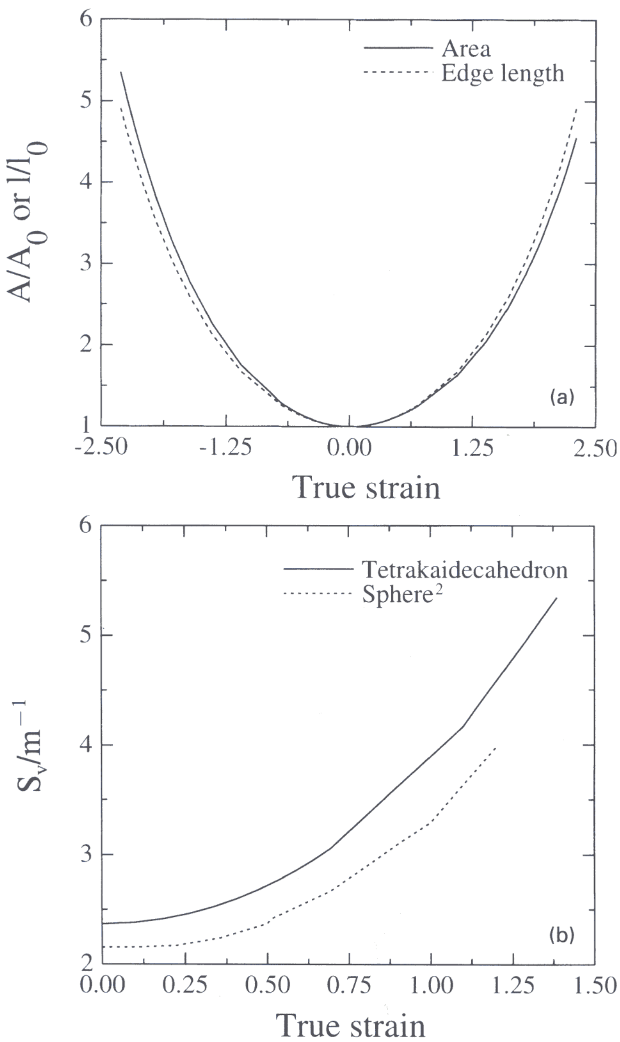
Similarly, the ratio of the total edge length of the deformed to undeformed tetrakaidecahedron is

$$\frac{l}{l_0}=\frac{1+b^2c+2(1+b^4c^2+2b^2c^4)^{1/2}}{6bc} \qquad (4)$$

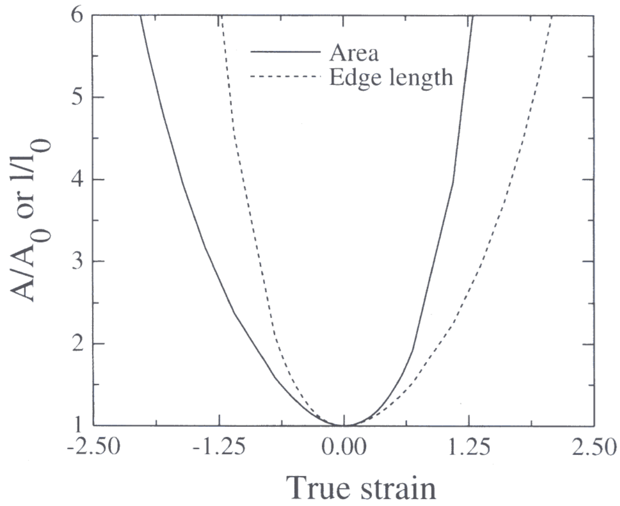


1 Shape of tetrakaidecahedron: coordinate axes illustrated are orthogonal with each basis vector of length *a*

These ratios are illustrated for plane–strain deformation ($b = 1/c$) in Fig. 2*a*, as a function of strain along the rolling direction. A negative value of the strain implies an antirolling deformation beginning with an equiaxed grain structure. The increase in the edge length is approximately



2 *a* increase in surface area and edge length of tetrakaidecahedron as function of strain along rolling direction during plane strain deformation: negative value of strain implies antirolling operation *b* comparison of surface per unit volume S_V for tetrakaidecahedron and sphere,[2] assuming that $a = 1$ and 1·393 m for tetrakaidecahedron and sphere respectively



3 Increase in surface area and edge length of tetrakaidecahedron as function of strain along radial direction during a wire drawing operation: positive value of strain implies antidrawing operation

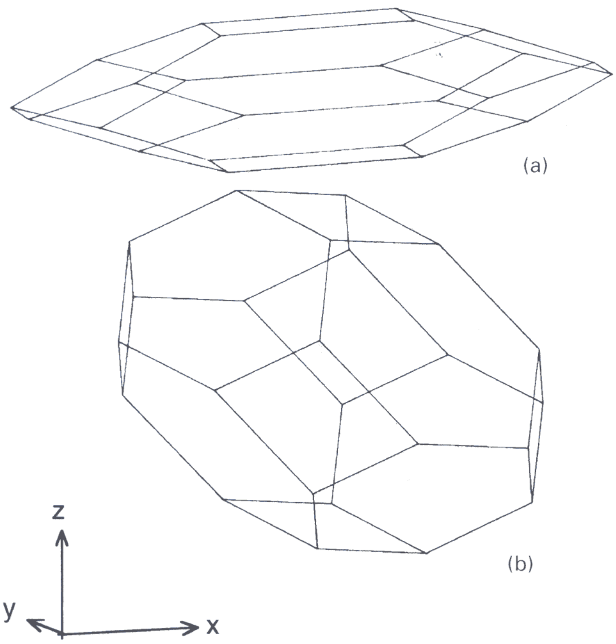
the same as that in the surface area. The negative value of strain signifies a compression along the third direction ($c < 1$). The increase is roughly symmetrical for the positive and negative values of strain, though equations (3) and (4) show that it cannot be precisely symmetrical. Comparison with the results of Umemoto *et al.*[2] in Fig. 2*b* shows that the tetrakaidecahedron naturally starts off with a larger surface area per unit volume when compared with a sphere. However, the rate at which the surface per unit volume S_V increases with strain is comparable for the two shapes. It should be noted that to enable a valid comparison, the volumes of the tetrakaidecahedron and sphere have been set to be equal for the calculations presented in Fig. 2*b*. Therefore, the dimension *a* is set at unity and 1·393 for the tetrakaidecahedron and sphere respectively.

Another type of deformation common in the processing of steel is wire drawing or rod rolling, characterised by $b = c$. The results for this are illustrated in Fig. 3, where the strain on the horizontal axis is along the radial direction (i.e. normal to the drawing direction). A positive strain therefore implies an antidrawing operation but always beginning with an equiaxed grain structure.

It is interesting to compare the results illustrated in Figs. 2 and 3. In both rolling and drawing, the main change in length is along the rolling or drawing directions respectively. Therefore, the rate at which the edge increases with strain is found to be similar for both deformations. The rate at which area increases with strain is larger for drawing deformation, because there is zero strain along one of the principal directions during plane strain rolling deformation.

Table 1 Six vectors which completely define edges of tetrakaidecahedron and their components after deformation S

Vector	Before deformation	After deformation
1	$[a \ 0 \ 0]$	$[ab \ 0 \ 0]$
2	$[0 \ a \ 0]$	$[0 \ ad \ 0]$
3	$\left[-\frac{a}{2} \ -\frac{a}{2} \ \frac{a}{\sqrt{2}}\right]$	$\left[-\frac{ab}{2} \ -\frac{ad}{2} \ \frac{ac}{\sqrt{2}}\right]$
4	$\left[\frac{a}{2} \ -\frac{a}{2} \ \frac{a}{\sqrt{2}}\right]$	$\left[\frac{ab}{2} \ -\frac{ad}{2} \ \frac{ac}{\sqrt{2}}\right]$
5	$\left[\frac{a}{2} \ \frac{a}{2} \ \frac{a}{\sqrt{2}}\right]$	$\left[\frac{ab}{2} \ \frac{ad}{2} \ \frac{ac}{\sqrt{2}}\right]$
6	$\left[-\frac{a}{2} \ \frac{a}{2} \ \frac{a}{\sqrt{2}}\right]$	$\left[-\frac{ab}{2} \ \frac{ad}{2} \ \frac{ac}{\sqrt{2}}\right]$



4 Tetrakaidecahedron after *a* plane strain deformation with a reduction of 50% along the *z* axis and *b* after wire drawing with reduction of 50% along *z* and *y* axes: *a* has been uniformly scaled down in size by a factor of 2 relative to *b*

Figure 4 shows the shape of the tetrakaidecahedron after a plane strain deformation and after a wire drawing type of deformation. These were generated from the coordinates of the vertices of the original tetrakaidecahedron using equation (2). The shape in Fig. 4*b* appears asymmetrical because the starting shape of the tetrakaidecahedron is not symmetrical relative to the *x* axis (the drawing direction) as is evident in Fig. 1.

Conclusions

Rigorous relationships have been derived for the increase in the surface area and edge length when equiaxed grains, idealised as space filling tetrakaidecahedra, are homogeneously deformed. This information should be of use in the modelling of transformation kinetics for reactions which are heterogeneously nucleated. The results improve on a previous model which was based on the deformation of a sphere.

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