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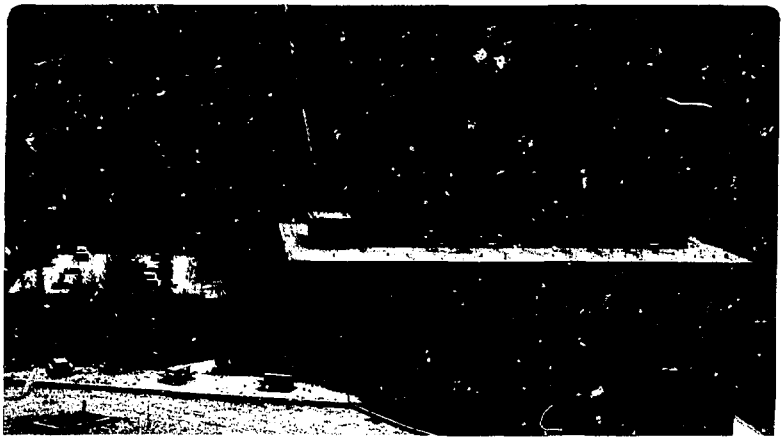

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COMPUTER SIMULATION OF THE MARTENSITE TRANSFORMATION IN A MODEL TWO-DIMENSIONAL BODY

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By

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Abstract

An analytical model of a martensitic transformation in an idealized body is constructed and used to carry out a computer simulation of the transformation in a pseudo-two-dimensional crystal. The reaction is assumed to proceed through the sequential transformation of elementary volumes (elementary martensitic particles, EMP) via the Bain strain. The elastic interaction between these volumes is computed and the transformation path chosen so as to minimize the total free energy. The model transformation shows interesting qualitative correspondencies with the known features of martensitic transformations in typical solids.

I. Introduction

It is widely recognized that many of the most interesting and least understood features of martensitic transformations reflect the need to accommodate the substantial internal elastic strains which develop as the transformation proceeds. Theoretical studies of the heterogeneous nucleation of martensite (1,2) have focused on the identification of crystal defects or distributions of defects whose strain fields may serve to relieve the large strain energy associated with a single-variant martensite nucleus. The more successful theories of the internal structure, shape, and habit of fresh martensite are crystallographic models (3,4) which are predicated on the assumption that the preferred martensite substructure, shape, and habit is that combination which most nearly insures a net invariant plane strain, the internal strain state which minimizes the elastic energy (5). Elastic effects are also believed to participate in the continuation of the transformation through the autocatalytic nucleation of sequential martensite plates, to influence the thermal characteristics of the transformation, and to affect the retention of high-temperature phase in "fully-transformed" product.

Given the prominence of elastic effects in the nucleation, growth, and morphology of martensite, tractable analytic models of the transformation which include elastic interactions should prove particularly fruitful in new theoretical insight. One such model has been under development by the authors for some time, and has recently been used to carry out computer simulation studies of martensitic transformations in simple systems (6).

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This model is briefly described and an example of its initial results presented in the following.

II. Model of the Martensite Transformation

The linear theory of elastic inclusions in anisotropic media, as developed by Khachaturyan (7), permits the straightforward computation of the elastic energy associated with an arbitrary distribution of inclusions under the assumption that the elastic constants are uniform. The relevant equations can be written so that the elastic energy is the sum of the self-energies of the inclusions plus a simple sum of binary interactions between them. The real-space form of the elastic potential which determines the binary interactions can be easily calculated. Moreover, the formulation insures a simple kinematics for a process involving the appearance of elastic inclusions since in a linear model a macroscopic inclusion may be regarded as the direct sum of elementary inclusions which make it up.

To construct a model of the martensite transformation based on the theory of elastic inclusions we refer the crystal to a superlattice whose Wigner-Seitz cells define elementary volumes which transform. Following the FCC→BCC transformation the parent lattice is assumed cubic and the Bain strain is taken to be tetragonal. In dyadic form

$$\underset{\sim}{\varepsilon}^{o}=\varepsilon^{o}_{11}(\underset{\sim}{e}_1\underset{\sim}{e}_1+\underset{\sim}{e}_2\underset{\sim}{e}_2) + \varepsilon^{o}_{33}\,\underset{\sim}{e}_3\underset{\sim}{e}_3 \tag{1}$$

where the $\underset{\sim}{e}_i$ are unit vectors along the cubic axes. A given tetragonal strain, specified by the values of ε_{11} and ε_{33}, yields three distinct variants of the elementary martensite particle which differ only in the selection of the tetragonal axis, $\underset{\sim}{e}_3$, from among the three cubic axes.

The distribution of EMP over the superlattice is described by the distribution functions $\zeta_p(\underset{\sim}{R})$ (p=1,2,3), which take the value one if there is an EMP of type p at $\underset{\sim}{R}$ and are zero otherwise. A configuration (α) of the body is defined by making a particular choice of the three $\zeta_p(\underset{\sim}{R})$. A configuration, α, may evolve to the immediately succeeding configuration, α+1, by adding an EMP of type p at any site $\underset{\sim}{R}$ which is unoccupied, or by deleting an EMP from any occupied site. The free energy change on either modification is (neglecting a chemical contribution to the surface energy) governed by the thermoelastic potential:

$$\phi^{\alpha}_{p}(\underset{\sim}{R})=N_o\Delta\mu + \Delta\phi^{\alpha}_{p}(\underset{\sim}{R}) \tag{2}$$

where $\Delta\mu$ is the chemical free energy change per atom, N_o is the number of atoms in an EMP, and $\Delta\phi^{\alpha}_{p}(\underset{\sim}{R})$ is the change in elastic energy

$$\Delta\phi^{\alpha}_{p}(\underset{\sim}{R})= \phi^{o}_{p} + \sum_{q}\sum_{\underset{\sim}{R}'}\omega_{pq}(\underset{\sim}{R}-\underset{\sim}{R}')\ \zeta_q(\underset{\sim}{R}') \tag{3}$$

The evaluation of the elastic self-energy ϕ^{o}_{p} and the binary potential $\omega_{pq}(\underset{\sim}{R})$ in terms of fundamental quantities is straightforward and is given in reference (6). If an EMP of type p at $\underset{\sim}{R}$ is eliminated the associated free energy change is $-\phi^{\alpha}_{p}(\underset{\sim}{R})$.

Given a configuration, α, the values of the thermoelastic potentials for the possible elementary changes in α, and the value of any inherent activation barrier, the mean and variance of the time required for the evolution of α through a thermally-activated process may be computed, and the particular elementary event causing the evolution of α may be chosen statistically. By iterating this procedure the kinetics and the "path" of the model transformation (i.e., the sequence of successive configurations) may be found. It is, in fact, only necessary to use computer simulation to determine the transformation path; the kinetics of transformation may be computed exactly once the path is known (6).

III. Example of a Transformation in Two Dimensions

To define a simple transformation case for computer simulation let the solid be a psuedo-two-dimensional body (in the sense that its elementary particles are infinite rods perpendicular to the representation plane), let the solid have isotropic elastic constants, and let the Bain strain be a simple shear involving an expansion along one of the axes of the two-dimensional grid and a compensating contraction along the other. In this case there are two variants of the elementary martensite particle which differ in orientation of the expansion axis. The elastic potential ($\omega_{pp}(\underset{\sim}{R})$) for the interaction of like particles is shown in Figure 1. By symmetry the interaction potential ($\omega_{pq}(\underset{\sim}{R})$) for unlike particles is the negative of the potential shown. The chemical driving force ($\Delta\mu$) is assumed to be a linear function of the undercooling (ΔT).

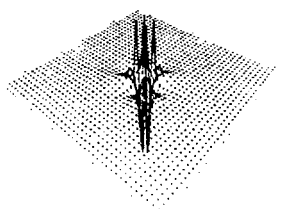

Fig. 1

Since the martensite transformation is known to be heterogeneously nucleated, we simulate the transformation of a defective lattice. For simplicity the pre-existing defects are taken to be a random distribution of elementary martensite particles. In the particular case illustrated here, ten such particles are randomly distributed over a 40x40 grid. We further assume that the transformation follows the "minimum energy path", determined by maximizing the energy decrease at each step and that the transformation can proceed only if the associated free energy change is negative, as follows naturally if the elementary martensite particle is very large or if the temperature at which the transformation occurs is very low.

Under the assumptions listed the martensitic transformation is athermal, and occurs progressively on continuous cooling. The variation of the fraction of martensite with undercooling, measured in energy units, is illustrated in Figure 2. The transformation is seen to initiate at an undercooling of approximately 0.09, and to reach completion at an undercooling of approximately 0.6. For comparison, the undercooling

required to homogeneously nucleate the martensite phase in this case is 0.6447.

The nucleation of the martensite transformation il illustrated in Figure 3. The transformation nucleates as a two-layer twinned plate, and grows along the (11) habit plane until it nearly closes on itself, as shown in Figure 4. However, before closing on itself the growing plate encounters the strain fields of other pre-existing defects, which causes the transformation to stop, to be resumed after further undercooling. This phenomenon illustrates the dual role of pre-existing defects. The strain fields of these defects promote the nucleation of martensite but interfere with its growth.

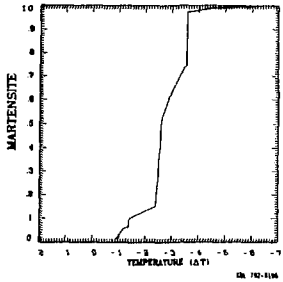

Fig. 2

Microstructures: ( )=Austenite, (-)=X-Martensite, (ı)=y-Martensite

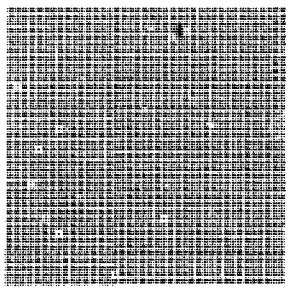

Fig. 3

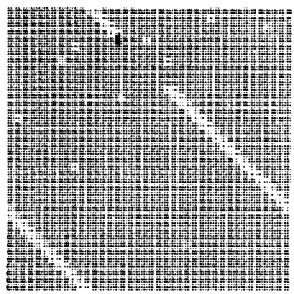

Fig. 4

The transformation develops further on decreasing temperature. Additional plates nucleate and grow, and may be oriented either parallel to or perpendicular to the original martensite plate. These autocatalytically nucleated plates sometimes initiate from pre-existing defects, and are sometimes homogeneously nucleated in defect-free regions of the lattice. Interestingly, the parallel martensite plates often form in an aggregate twin orientation to one another with a layer of retained austenite in the intervening space. An intermediate stage

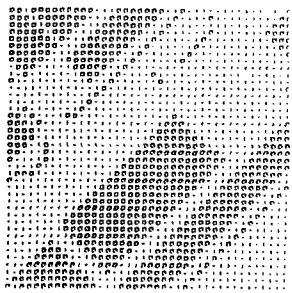

Fig. 5

in the transformation illustrating some of these features is shown in Figure 5. As the transformation nears completion, only a small residue of isolated austenite particles is retained. This residue of austenite is extremely stable, and a large undercooling is required to eliminate it and bring the transformation to completion.

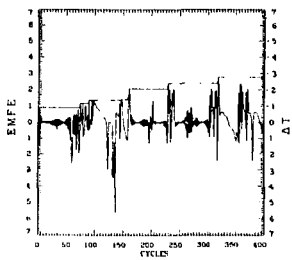

Figure 6

The energetics of the transformation are illustrated in Figure 6, which shows the magnitude of the chemical driving force as a horizontal line, and the magnitude of the elastic energy per step as an oscillating function for the first 400 transformation steps. The elastic energy is a noisy function which oscillates about the value zero. The transformation is stopped by occasional, large excursions from the value zero which exceed the chemical driving force. These excursions identify the nucleation steps along the transformation path. They are responsible for the progression of the martensite transformation through a sequence of transformation bursts as the temperature is lowered, and the chemical driving force raised.

IV. Conclusion

A model of the martensitic transformation in a simple system has been developed which allows the transformation to occur through the sequential appearance of elementary volumes of martensite in the parent matrix and accounts for the energetic contribution of the elastic interaction between these elementary volumes. The model has been used for the computer simulation of a martensitic transformation in two dimensions. Despite the simplicity of the model, the features observed in the simulated transformation are encouragingly real. The initial martensite phase is heterogeneously nucleated and grows as a twinned plate along a definite habit plane. The overall transformation occurs through a series of bursts which are sequentially triggered as the temperature is lowered. These bursts involve the autocatalytic nucleation and growht of martensite plates which may parallel or branch with respect to the original plate. Bands of retained austenite are occasionally observed between parallel plates which are in an aggregate twin-orientation to one another. Residual austenite is retained to a very late stage in the transformation, and is elastically stabilized to the extent that very large undercoolings are required to eliminate it.

Acknowledgement

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