Multiple, Simultaneous, Martensitic Transformations: Implications on Transformation Texture Intensities

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Abstract. A theory is developed for martensite variants that have different start temperatures but exist in the same steel. The method enables the volume fractions of each kind of martensite to be followed as a function of the steel temperature. The problem is relevant to the calculation of detail in transformation texture when phase changes occur under the influence of external stress. It should allow for the first time, the estimation of both the location of crystallographic poles on a stereographic projection, and the diffraction intensity associated with that location. It is found that the increment of transformation as a function of undercooling is identical for all variants, once simultaneous transformation begins. Any variance in the absolute fractions is due to the differences in the martensite-start temperature.

Introduction

It is now necessary to think of a way of dealing with the kinetics of austenite decomposition into more than one kind of martensite, albeit with the same crystal structure but different thermodynamic stabilities. Such transformations may occur simultaneously when appropriate undercoolings are achieved, but the motivation of the work lies in an entirely different context, that of calculating transformation plasticity.

Motivation

There are important unresolved difficulties in the calculation of crystallographic texture due to displacive transformation under the influence of stress [1, 2]. It is often assumed that it is sufficient to plot calculated crystallographic orientations on stereographic projections or similar devices, and then compare against experimental data which contain not only the location of poles but also the associated diffraction intensity. This is misleading because crystallography on its own predicts only the positions of the poles. The implicit assumption is that all variants, even those that oppose external influences, contribute equally to intensity. This is illustrated in the austenite grain of Fig. 1a; two variants of martensite of equal size will display the same calculated texture as that in which one variant is a hundred times larger in volume than the other. The correct scenario is that illustrated in Fig. 1b, where the density of poles is much larger in the case of the dominating variant.

The estimation of intensity requires thermodynamic and kinetic theory. The total free energy that a particular variant of martensite experiences when transformation occurs under the influence of stress determines whether or not the formation of that variant is favoured. Of the 24 possible orientations of martensite that can form in any given grain of austenite, some will be favoured and others opposed since they do not comply with the stress - in other words, *variant selection* occurs. The total free energy is the sum of the chemical and mechanical components, the latter being zero in the absence of an applied stress during transformation [3, 4]:

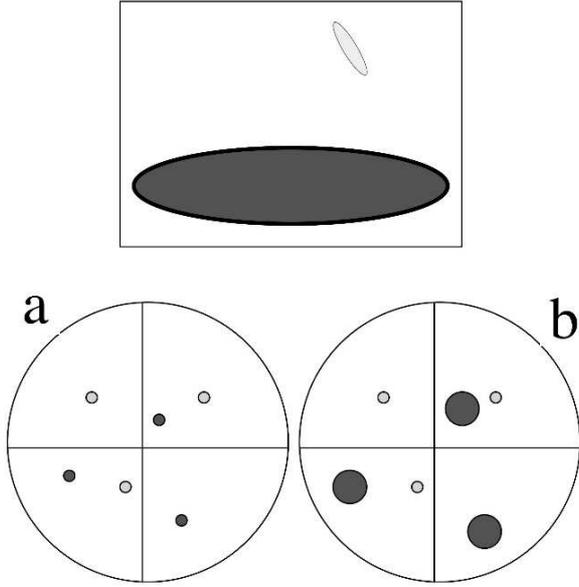$$\Delta G = \Delta G_{CHEM} + \Delta G_{MECH} \tag{1}$$

Fig. 1: Schematic illustration of the difficulty in calculating pole figures. Note that the size of the dots is intended to reflect the density of poles. (a) Representation of pole figure calculated without taking account of the volume of the diffracting crystal. (b) Intensity scaling with the fraction of the contributing crystals. Any method which only plots crystallographic orientations in comparisons against experimental data will therefore be incomplete.

where for an applied stress that is uniaxial, $\Delta G_{MECH} = s\tau + \delta\sigma_N$ [3], s and δ representing the shear and dilatational strains due to transformation, the latter being normal to the martensite habit plane. The magnitudes of the shear stress τ on the habit plane, and σ_N normal to that plane, depend on the orientation of the plate relative to the applied stress. Therefore, the sign and magnitude of the mechanical driving force depends on the orientation of each of the 24 variants of martensite in any given grain of the parent phase with respect to the external stress. Strong variant selection occurs when the ratio of $\Delta G_{MECH}/\Delta G$ is large [5], as illustrated in Fig. 2, which is empirical in the sense that we do not know whether this relationship should be linear [6].
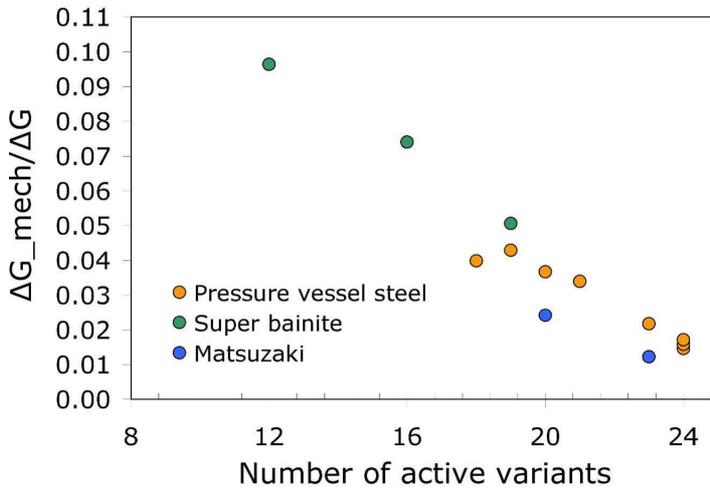

Fig. 2: $\Delta G_{MECH}/\Delta G$ versus the number of most favoured variants per grain (n), for a variety of steels. [6]. Data from [7, 8, 6].

An important point to note is that during transformation under stress, the martensite-start temperature is different for each of the 24 crystallographic variants in any given grain. This is because transformation is triggered only when $\Delta G < \Delta G_{M_S}$, where ΔG_{M_S} is a critical value of the free energy change.

There are therefore, 24 values of M_S to deal with for each austenite grain, and a theory is necessary to enable the volume fractions of each of these variants to be estimated as a function of temperature.

Kinetic theory for single variety of martensite

We now proceed to describe how the volume fraction of each variant of martensite, with its distinct martensite-start temperature, might be calculated. The basic theory has its origins in the empirical equation derived by Koistinen and Marburger [9] and elaborated by Magee [10]. Consider first the case of stress-free transformation where a unique M_S is defined for a given steel. Following Magee, the number dN of new plates per unit volume of austenite is assumed to increase linearly with the increment in ΔG due to undercooling below M_S:

$$dN = -\phi\, d\{\Delta G\} \qquad \text{where } \phi \text{ is a constant.} \tag{2}$$

The change df in the fraction of martensite, given an average volume per plate of $\overline{V}$ is

$$df = \overline{V}(1 - f)\, dN \tag{3}$$

since $(1 - f)dN$ is the change in the per unit volume of sample. On combining these equations and making the substitution

$$d\{\Delta G\} \equiv \frac{d\{\Delta G\}}{dT} dT$$

we see that

$$df = -\overline{V}\phi(1 - f)\frac{d\{\Delta G\}}{dT} dT \tag{4}$$

that on integration gives the classical Koistinen and Marburger equation with $\chi \approx -0.011$:

$$1 - f = \exp\left[\underbrace{\overline{V}\phi\frac{d\{\Delta G\}}{dT}}_{\chi = -0.011}(M_S - T)\right]. \tag{5}$$

Simultaneous formation of multiple martensite varieties

From Eq. 4 we see that $df = \chi(1 - f)\, dT$. This relationship can be generalised in much the same way that the original Avrami theory [11, 12, 13] for overall transformation kinetics was adapted for simultaneous transformations [14, 15, 16, 17, 18]. So for two different martensitic reactions happening at the same time, and in a temperature interval dT

$$
\begin{aligned}
df_1 &= \chi(1 - [f_1 + f_2])\, dT, &\text{with} &\quad df_1 = 0 \quad \text{if} \quad M_{S_1} < T \\
df_2 &= \chi(1 - [f_1 + f_2])\, dT, &\text{with} &\quad df_2 = 0 \quad \text{if} \quad M_{S_2} < T
\end{aligned}
\tag{6}
$$

These equations can be numerically solved as a function of undercooling below the respective M_S temperatures. Some calculations are illustrated in Fig. 3. Notice that at the point where the two kinds of martensite start to form together, the increments df in their respective fractions as a function of undercooling dT are identical, consistent with Eq. 6. This is because it is assumed that χ is the same for both 'phases'. This parameter is of course determined by the mean volume per plate $(\overline{V})$ and $(\Delta G)/dT$. Since the only thermodynamic difference between the two forms of martensite comes from the mechanical free energy term ΔG_{MECH}, which does not vary with temperature, $d\{\Delta G\}/dT = d\{\Delta G_{CHEM}\}/dT$ so that χ does not depend on the M_S temperature of the variant.

Similarly, if the geometrical partitioning of the austenite remaining once M_{S_2} is reached is identical for all variants, then χ can reasonably be assumed constant. The conclusion therefore, is that following the onset of simultaneous transformation of the kind described here, the change in volume fraction of each variant of martensite is *identical*. Differences in the total volume fractions of individual variants arise only through the thermodynamic effect of the mechanical driving force on the martensite-start temperature.
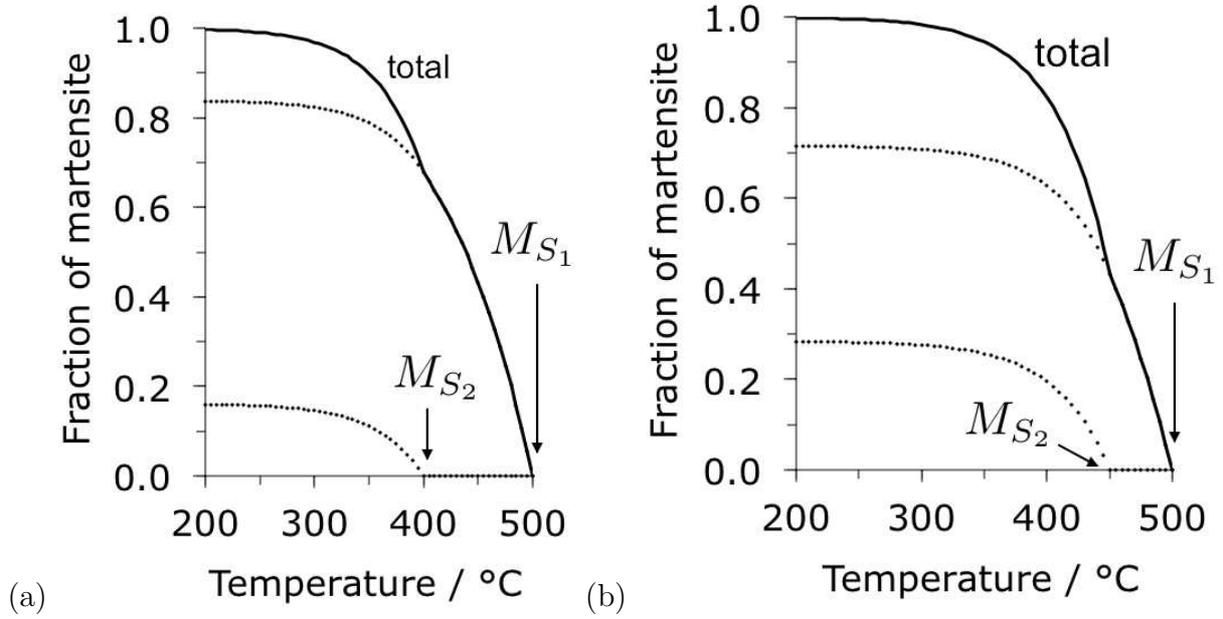

Fig. 3: Two martensite-start temperatures, (a) 500°C and 400°C, (b) 500°C and 450°C .

There are circumstances in which the applied stress can vary with temperature, for example during the cooling of a mechanically constrained tensile specimen of austenite. It cannot then be assumed the χ will be identical for each variant. Fig. 4 illustrates a case where χ depends on variant. In such a case, the value of χ should include the temperature dependence of the mechanical driving force through the term $d\{\Delta G\}/dT \equiv d\{\Delta G_{CHEM} + \Delta G_{MECH}\}/dT$ in equation 5. So the ordinary value of $\chi = -0.011$ which is identical for all variants, would be modified to the new value χ^i as follows:

$$\chi^i = \chi \times \frac{d\{\Delta G_{CHEM} + \Delta G^i_{MECH}\}/dT}{d\{\Delta G_{CHEM}/dT\}} \tag{7}$$

where the superscript i refers to the particular martensite variant of interest.

Summary

A simple theory is presented to permit the calculation of the volume fractions of martensite variants which differ in their martensite-start temperatures within the same austenite grain or in a sample of polycrystalline steel. It is found that the differences in volume fractions obtained can be attributed entirely to variations in M_S. Once the variants of martensite grow together, the increments in each of their volume fractions as a function of an increase in undercooling, are identical.

This theory forms the basis for predicting the diffracted intensities observed during the development of transformation texture under the influence of external stress.
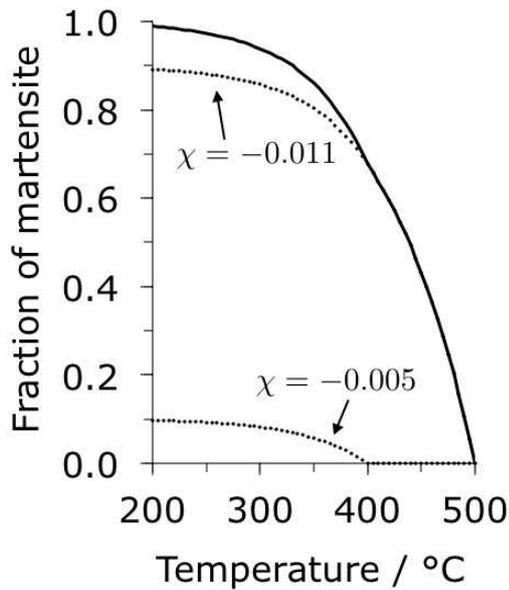
Fig. 4: This figure corresponds to Fig. 3a, but with the Koistinen and Marburger parameter χ taken to be different for the two variants of martensite. The total fraction of variant 2 is therefore, significantly reduced.

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