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U. Dahmen and K.H. Westmacott

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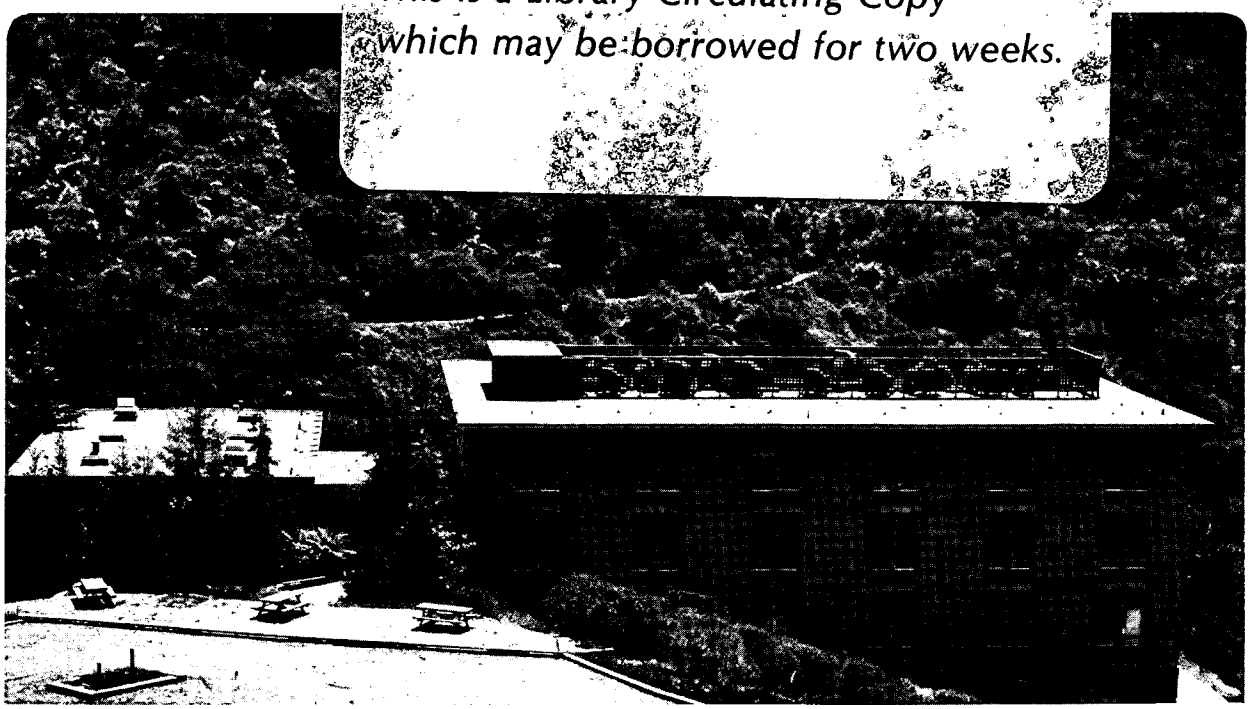

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U. Dahmen and K.H. Westmacott

The Accommodation of Precipitate Plates Modelled as a Tensile Test

National Center for Electron Microscopy
Materials and Chemical Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

Synopsis

Thin plate precipitates in transformations with principal strains of mixed sign are approximately in a state of uniaxial stress if the interface contains an invariant line. This similarity to a tensile test can be used for the prediction of coherent and semicoherent plate habits; to relieve the uniaxial stress the tensile axis must lie in an elastically soft direction for coherent plates and at approximately 45° to the operative slip system for semicoherent plates. The habit plane is the plane that contains both the invariant line and the tensile axis. Predictions of this simple model are shown to be in excellent agreement with available experimental observations on plate precipitates in several bcc interstitial alloys.

Introduction

The orientation relationship and the corresponding morphology of precipitates in a matrix phase are crucial factors in the link between microstructure and properties of materials. In the case of coherent inclusions (precipitates) considerable success has been achieved in the prediction of precipitate shapes and habits through the application of classical elastic continuum theory(1-5). While this approach offers the advantages of mathematical rigor, application of the results to practical situations is sometimes difficult.

A complementary approach is to seek to understand the physical principles underlying different classes of phase transformation and express the results in a simplified form, readily useable by the practitioner. This method has been used successfully to describe precipitate morphologies and orientation relationships for a wide variety of alloy systems(6-9). In the present contribution the results for the case of

coherent and semicoherent precipitate plates in transformations with principal strains of mixed sign are derived. This is followed by a comparison of the predictions of the model with experimental observations by TEM, which shows excellent agreement.

Underlying Principles

It is possible to point to some simple physically plausible principles that can help understand and predict basic particle morphologies and orientation relationships. For example it is generally true that precipitate dimensions tend to be inverse to their transformation strain, i.e., largest in the direction of smallest strain and vice versa[10]. This is the case for elastic strain accommodation of coherent inclusions as well as plastic accommodation of semicoherent precipitates. The modifying influence of crystal anisotropy[11-14] is significant only when the transformation strain is isotropic or nearly isotropic, e.g., a pure dilatation. In most other cases it is the anisotropy of the transformation strain that determines the shape. This is because the coherent strain energy and the semicoherent interface energy depend roughly on the square of the transformation strain. The prediction of precipitation shapes for transformations with principal strains of unmixed sign is thus quite straightforward. If one of the principal strains, e_3, is large and the other two, e_1 and e_2, are small and equal, the strain has cylindrical symmetry and a thin plate would be expected, as shown in Fig. 1a. However, if the principal strains are of mixed sign, as is the case in many alloy systems, the prediction of morphologies becomes more complex for both coherent and semicoherent precipitates. The present contribution outlines a simple model to predict and understand the orientation of a precipitate plate for this case of mixed principal strains.

Coherent Plates

An example of a transformation with mixed principal strains is an expansion e_3 in the [001] direction and a contraction $e_1=e_2$ in the (001) plane, as shown in [010] projection in Fig. 1c. An unextended line can be found at an angle θ to the (001) plane where $\tan\theta = \sqrt{-e_1/e_3}$. If a coherent precipitate plate is oriented to contain an unextended line in the interface, as seen in Fig. 1d, the state of stress within the plate is approximately the uniaxial stress shown in Fig. 1e, instead of the plane stress shown in Fig. 1b. The strain energy of a plate under uniaxial stress is only about one third of that under plane stress[8,12]. Thus one will always expect to find coherent plates with mixed principal strains inclined rather than normal to the plane of the unique principal strain.

This is the condition of an invariant (unextended and unrotated) line in the interface, as it is used for instance in martensite theory [e.g. 15]. To a good approximation this invariant line condition can predict plate precipitate habit planes if the remaining uniaxial stress in the plate is minimized. For coherent plates this is achieved if the tensile axis is a direction of small principal strain. If two principal strains are equal, the tensile axis must be a direction of low elastic modulus. For semicoherent plates the tensile axis must have a high resolved shear stress on the operating slip system. These simple principles will be examined in more detail below followed by applications to known alloy systems.

First, it must be pointed out that for the elastic case an improved condition is that of a stress-free rather than a strain-free direction. This changes the expression for the angle of inclination θ from $\tan\theta = \sqrt{-e_1/e_3}$ to $\tan\theta = \sqrt{-(1+\upsilon)e_1/(e_3+\upsilon e_1)}$, where υ is Poisson's ratio[8,17]. However, the correction is usually small enough to lie within experimental error of coherent habit plane determinations. In most cases it is therefore sufficient to use the simple invariant line condition.

If all three principal strains are different (and of mixed sign) the invariant line will lie between the two extreme principal strains and the tensile axis will be oriented along the smaller of the two unmixed principal strains[12]. If the two principal strains of unmixed sign are equal ($e_1 = e_2$), as for example in a cubic-to-tetragonal transformation, the tensile axis in the plate could be any direction in the (001) plane containing the uniform strain $e_1=e_2$. The final precipitate would be a plate inclined by $\theta°$ about this direction. In Fig. 1 (d and e) this was chosen arbitrarily to be [010]. In an anisotropic crystal this tensile axis should lie in a soft direction in the (001) plane to lower the strain energy further. The problem of minimum strain energy is then reduced to finding the direction $\underline{\rho}$ in the (001) plane with the smallest Young's modulus $E(\underline{\rho})$. This direction will become the tensile axis in the inclined precipitate under uniaxial stress. For directions in an (001) plane of an anisotropic cubic crystal, it can easily be shown that the <100> directions are soft if the anisotropy ratio $A > 1$ and <110> are favored if $A < 1$[8,12,18]. Since the tensile axis is contained in the habit plane and consititutes the axis of rotation for the plate, the minimum energy plate will lie on a plane of the type {okl} with $k/l \cong \sqrt{e_1/e_3}$ if $A > 1$. If $A < 1$, the habit plane will be of the type {hhl} with the same angle θ of inclination. Since the strain energy is mainly due to the elastic distortion of the inclusion, A should be strictly the anisotropy ratio of the precipitate.

Rigorous derivations of the conditions given above[11-14] and solutions for the less restrictive case of thick plates[5,19] can be found in the literature.

Semicoherent Plates

The tensile test analogy is particularly useful in describing the loss of coherency. Consider a thin plate in a state of uniaxial tension. If it deforms plastically it is most likely to do so on the slip system with the highest resolved shear stress. This depends on the relative position of the tensile axis and the slip system; and the resolved shear stress is a maximum if both the slip plane and the slip direction make an angle of 45° with the tensile axis. The problem of finding a direction in the (001) plane with a low Young's modulus in the elastic case now translates to finding the tensile direction in the (001) plane with the highest Schmid factor $R = \cos\phi \cos\lambda$ (where ϕ and λ are the angles of the tensile axis with the slip direction and the slip plane normal, respectively) for an available slip system. For a given slip plane the slip direction is linked to the tensile axis by the geometrical restriction of maintaining an unrotated and undistorted habit plane. The calculation of the slip direction is a lengthy process and as a first approximation it may be assumed that the Schmid factor is maximized when the tensile axis makes an angle of $\lambda = 45°$ with the slip plane. This geometry is illustrated schematically in Fig. 2a and b, and a dark field electron micrograph of an extracted semicoherent plate (γFe_4N) showing shear faults on a slip plane at approximately 45° to the plate is shown in Fig. 2c. Figures 3a and b show stereographically that for slip on the (101) or (110) planes the tensile axis at 45° to the slip plane is [100]. Together with the invariant line at the intersection of the cone of unextended lines with the slip plane this defines the habit plane which for these two cases must be of the type {okl}. For comparison the same situation for coherent precipitates is shown in Fig. 3c. Note that here the invariant line and the tensile axis lie at right angles, but the coherent tensile axis is [100] only for anisotropy ratios $A > 1$, while for $A < 1$ it is [110].

The stereograms in Fig. 3 illustrate the three different geometries used in comparing the model with available experimental data, although for some of the transformations ($e_1=e_2=e_3$) the cone of unextended lines will not be circular, but elliptical. Also, it must be kept in mind that even though the slip planes and the soft tensile axes are expressed in terms of crystal directions of the matrix crystal, the important properties are those of the corresponding directions in the precipitate crystal. Thus the elastic constants or slip geometry in the precipitate determine the habit planes, and the discussion in terms of the matrix is only a convenient tool.

Comparison with Experimental Observations

Table I compares the predictions of the model with selected reliable experimental observations available in the literature. It can be seen that in most cases straightforward application of the principles outlined above leads to good agreement

with experiment. Any apparent disagreement can be understood in terms of groups of variants or transformation twins. This phenomenon is perhaps most visible for Fe-N alloys. The {049} plates predicted for $\gamma' Fe_4N$ precipitates in Fe are actually found in groups of two mirror-related variants joined together in a butterfly-like morphology[9,20,21]. In a similar manner many segments of coherent $Fe_{16}N_2$ plates, all inclined by a predicted angle of ~9° to the (001) plane are joined together in a puckered sheet with an average habit plane of (001)[22]. TaO_y in Ta exhibits similar behavior; two (101) twin-related variants of the orthorhombic precipitate are arranged back-to-back to form an {032} habit plane[23]. This agrees with both the prediction for the untwinned coherent case where the elastic anisotropy determines the type of habit and with the prediction for the semicoherent case where (101) twinning is the deformation mode[5,23]. Similarly the observed {227} habit of V_2H agrees with the predictions for a coherent elastically anisotropic plate but observations show dislocations in the interfaces[24]. It has been shown that the {227} habit for a semicoherent plate corresponds to slip on a {112} plane[25], a case not shown in Fig. 3 but physically plausible and geometrically necessary for an {hhl} type habit.

Finally, the example of HfN on (001) planes in Mo[26,27] was included to illustrate that precipitates are inclined only when the principal strains are of mixed sign. For the unmixed strains of HfC, ZrN, ZrC and Hfc in Mo, the rule that precipitate dimensions tend to be inverse to the strain must be employed and leads to simple (001) habits[26]. This condition applies to a large class of alloy systems in which plates precipitate on low-index habit planes.

Most of the precipitation systems considered have been analyzed before using either martensite, or elasticity or O-lattice theory. The present contribution points out the underlying physical principles and gives a very simple method for predicting plate precipitate habit planes. Some of the approximations and their implications have been discussed elsewhere[8,17] but as shown in the examples in Table I they do not significantly affect the accuracy of the predictions, making this a useful method for the practical analysis of precipitation reactions.

Summary

-In its optimum orientation a plate shaped precipitate formed in a transformation with principal strains of mixed sign contains an invariant line in its interface.

-If coherent such a thin plate is in a state of uniaxial stress, similiar to a tensile test.

-This stress is relieved by selecting, within the geometric constraints, a tensile axis that is elastically or plastically soft.

-The habit plane is defined by the invariant line and the tensile axis.

-The predictions of this simple model are in good agreement with available experimental observations.

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Table I

Comparison of Predicted and Observed Habit Planes

System		γFe_4N-Fe	TiN-Mo	TiC-Mo	TaO_y-Ta	$\alpha''Fe_{16}N_2$-Fe	βV_2H-V	Mo_2C-Mo	HfN-Mo
Precipitate	structure	fcc	fcc	fcc	orthorhombic		bct	bct	hcp
	a	0.3795	0.423	0.432	0.3271	0.2861	0.3002 ± 0.001	0.3002	0.452
	b				0.3201				
	c				0.3610	0.3146	0.3302 ± 0.001	0.4724	
Matrix	structure	bcc	bcc	bcc	bcc	bcc	bcc	bcc	bcc
	a	0.2868	0.3147	0.3147	0.3322	0.2868	0.3032	0.3147	0.3147
Principal Strains	e_1	-0.064	-0.050	-0.030	-0.015	-0.002	-0.010	0.172	0.016
	e_2	-0.064	-0.050	-0.030	-0.036	-0.002	-0.010	0.064	0.016
	e_3	0.323	0.344	0.371	0.087	0.097	0.089	-0.043	0.436
Anisotropy	A				1.56	2.38	0.78		
Slip plane		101	101	101	101		112	110	
Inv. Line		494	252	131	032/232	071	031/131	113	none
Tensile Axis		100	100	100	100	100	110	100	100/ 010
Habit	predicted	049	025	013	023	017	114-227	031	001
	observed	049	~013	013	023	017/001	227	031	001
References		8,9	26	26	23	8,9,14,19	5,24,25	6,8	26,27

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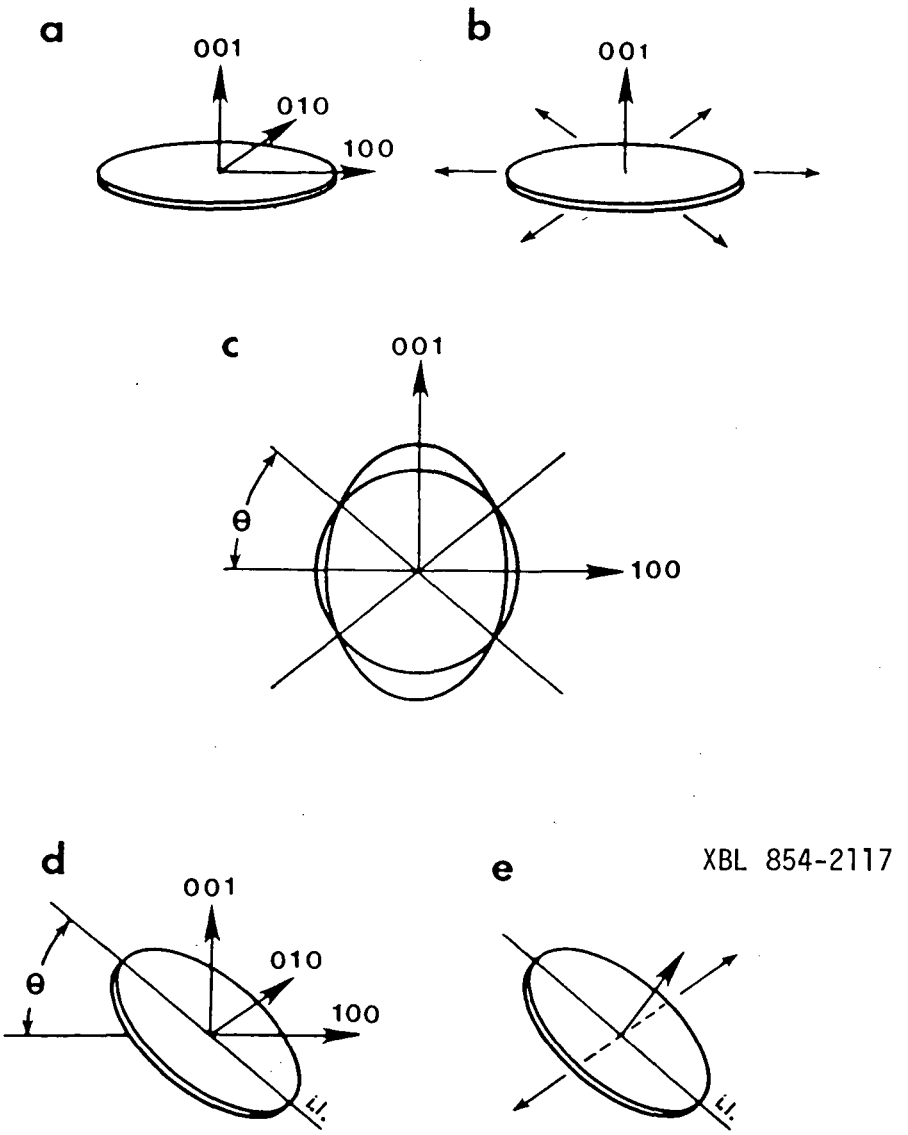
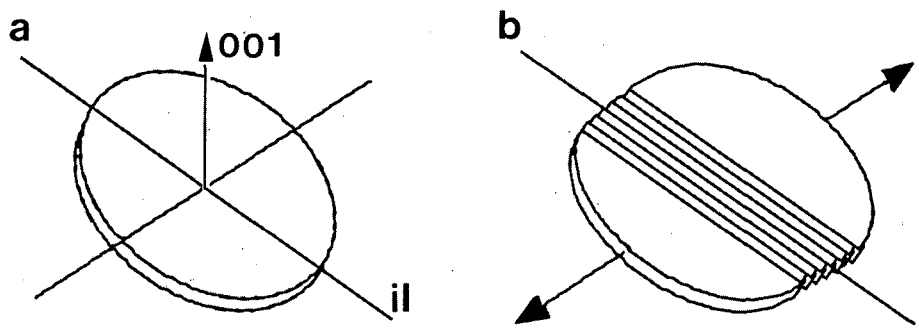


Fig. 1. (a) Thin plate precipitate on the (001) plane and (b) its state of plane stress. (c) The transformation strain is depicted schematically in the [010] projection with unextended lines at an angle θ to the (001) plane. In its optimum orientation (d) the thin plate is inclined and contains an invariant line in the interface. Its state of uniaxial stress along [010] is illustrated in (e).



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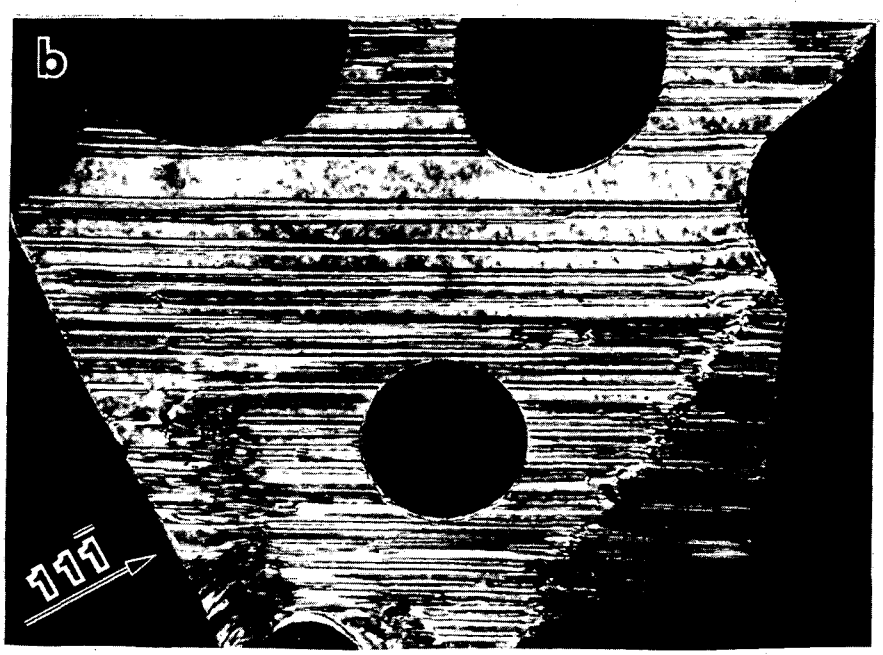

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Fig. 2. Illustration of tensile test analogy showing coherent plate under uniaxial stress in (a), loss of coherency by plastic yielding in (b) and dark field electron micrograph of extracted semicoherent precipitate plate ($\gamma' Fe_4N$) with shear faults in (c).

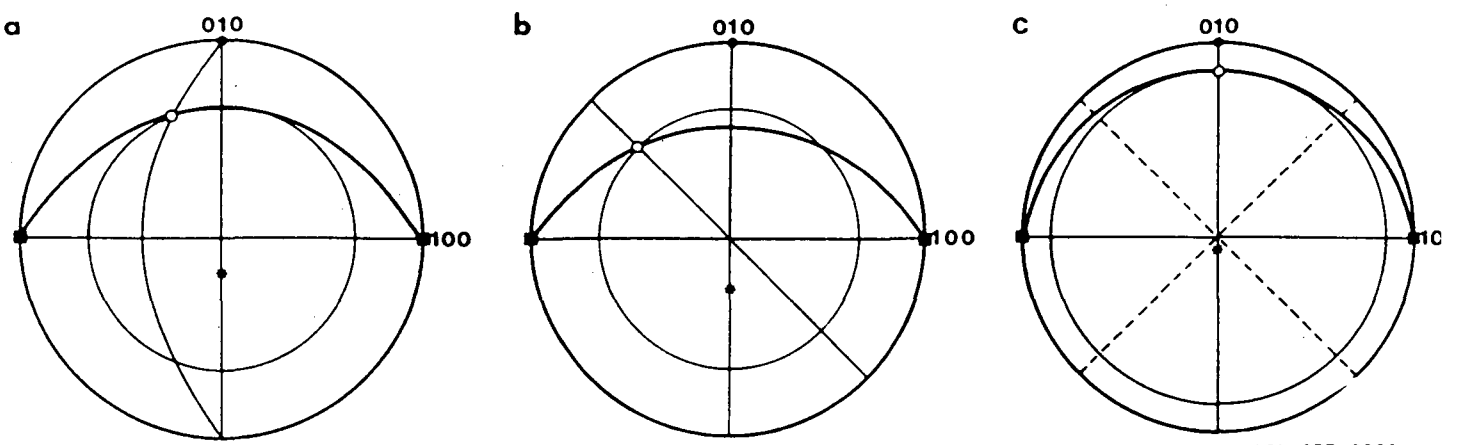

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Fig. 3. [001] Stereograms showing habit planes determined by the [100] tensile axis (solid square) and the invariant line (open circle) at the intersection of the cone of unextended lines with the inclined (101) slip plane in (a) and the vertical (110) slip plane in (b). The habit plane poles are marked by a star. The coherent case for A > 1 is illustrated in (c).

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