

lead to significant errors in the determination of lattice parameters.

The stacking fault probability is high, and every third or fourth plane contains a stacking fault. The GdCo<sub>2</sub> lattice (Structurbericht C15) is an fcc lattice containing eight atoms per unit cell. The cobalt atoms lie in sheets parallel to the {111} planes. For such an fcc structure the stacking faults lie in the {111} planes. Thus a high proportion of cobalt atoms lie in regions containing stacking faults and experience hyperfine fields which differ from those which one would expect for a perfect crystal. At the time of writing no GdCo<sub>2</sub> specimen has yielded a unique hyperfine field in a pulsed nuclear magnetic resonance experiment.

Assuming that the spacing between stacking faults is approximately three times the {111} interplanar spacing one can use Ayling's data for the yield strength to estimate the stacking fault energy. A value of about  $2 \times 10^{-4} \text{ J m}^{-1}$  results from such a calculation. This is comparable with the value calculated for GdFe<sub>2</sub> using similar assumptions.

In this paper we have established that it is necessary to consider the possibility of crystallographic sources of line shifts as well as the well known mechanical sources of line shifts if a

proper assessment of lattice parameters is to be made.

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## *The stability of equilibrium surface topography developed by sputtering*

In a series of recent papers the present authors and others [1] have considered the development of topography upon isotropic, homogeneous solids resulting from the variation of erosion rate induced by energetic ion sputtering as a function of the angle of incidence of the ion flux. These studies have shown that a steady state topography will develop after high fluence irradiation where the surface is either (a) planar or (b) faceted, with facet angles inclined at  $(\pi/2) - |\theta_p|$  to the ion flux incident direction, but except in the case of computational simulation [2, 3] have not distinguished the relative stability of these end forms. It is the purpose of this communication to explore the stability criteria.

As in earlier studies [1] we assume a surface generator in the xOy plane to be irradiated with a

uniform ion flux  $\Phi$  in the  $-y$ -direction. If the sputtering yield (number of atoms eroded per incident ion) is denoted by  $S$ , then, frequently, the variation of  $S$  with the angle  $\theta$  between the ion flux and the normal to a surface element, is given by the functional form shown in Fig. 1a, i.e.  $S = S_0$  at  $\theta = 0$ , rising to maxima at  $\theta = \pm \theta_p$  and declining, thereafter to  $S = 0$  at  $\theta = \pm(\pi/2)$ .

If the surface generator is described, at time  $t$ , by the form

$$y(t) = f(x, t) \quad (1)$$

then, in order that this generator should maintain a time independent profile, Equation 1 must satisfy the general equation of motion for a wave, travelling in both  $x$ - and  $y$ -directions, with constant shape (the "soliton" [4, 5] solution), i.e.

$$y + v_y \cdot t = f(x - v_x \cdot t) \quad (2)$$

$v_x$  and  $v_y$  are the velocities of motion of the wave in  $x$ - and  $y$ -directions respectively.

Differentiation of Equation 2 with respect to  $x$  or  $t$ , and noting that  $\tan \theta|_t = dy/dx|_t$ , then leads to the relation

$$\frac{\partial \theta}{\partial t} \bigg|_x \bigg/ \frac{\partial \theta}{\partial x} \bigg|_t = -v_x \quad (3)$$

and similar operations with respect to  $y$  and  $t$  lead to

$$\frac{\partial \theta}{\partial t} \bigg|_y \bigg/ \frac{\partial \theta}{\partial y} \bigg|_t = v_y \quad (4)$$

Comparison of these requirements with the defining equations of motion [1] of the surface during sputter erosion lead to the identities

$$\frac{\Phi}{N} \frac{dS}{d\theta} \cos^2 \theta = v_x \quad (5)$$

$$\frac{\Phi}{N} \left( \frac{dS}{d\theta} \sin \theta \cos \theta - S \right) = v_y \quad (6)$$

where  $N$  is the solid atomic density.

Equations 5 and 6 indicate that, in order for the surface contour to remain of time independent shape, both the quantities  $(dS/d\theta)\cos^2\theta$  and  $(dS/d\theta)\sin\theta\cos\theta + S$  must be constants. These parameters are plotted in Figs. 1b and c, as a function of  $\theta$ , for the general  $S/\theta$  form given in Fig. 1a. It is clear, from these figures, that the requirements of Equations 5 and 6 can be fulfilled for any single and constant value of  $\theta$ , i.e. a straight line (or planar surface) configuration. Fig. 1b also indicates that profiles consisting of two linear segments (at  $\theta_1, \theta_2$  where  $v_{x_1} = v_{x_2}$ ) may also retain constancy of form, but Fig. 1c indicates that this is fallacious since, except for special values of  $\theta$ , nowhere does  $v_{x_1} = v_{x_2}$  and  $v_{y_1} = v_{y_2}$  simultaneously. These special circumstances are  $\theta = \text{everywhere}$  and  $\theta = \pm\theta_p$ . This indicates that the *only* possible equilibrium end forms are flat surfaces, normal to the ion flux, and faceted surfaces with semi-vertical angles  $(\pi/2) - |\theta_p|$ . For all other combinations of  $\theta_s$ , shape continuity is not preserved, particularly when both positive and negative values of  $\theta$  are contained in the end form. The  $\pm\theta_p$  configuration

may be obtained as either a planar "sawtooth" faceted structure or a collection of cones or pyramids of semi-vertical angles  $(\pi/2) - |\theta_p|$ . It is notable that a combination of  $\theta = 0$  and  $\pm\theta_p$  is not acceptable so that isolated cones or pyramids upon a flat surface are only transient artefacts, whereas if a *whole* surface is faceted, or cone covered with  $\theta = \pm\theta_p$ , there may be a more permanent structure. Such a cone or pyramid "forest" has been observed [6] on an isolated grain in  $\text{Ar}^+$  ion-bombarded Cu.

Although the above considerations indicate necessary conditions for shape invariancy, they do not allow a decision as to which of the only two end forms ( $\theta = 0$  or  $\theta = \pm\theta_p$ ) is the more stable. In order to postulate such "sufficient" conditions for "stable equilibrium", we note that since the wave velocities are functions of angle  $\theta$ , then it would be expected that following a perturbation from a stable structure there would be an eventual return to the stable structure if the velocities were minimized relative to angular perturbations, i.e.  $dv_x/d\theta = dv_y/d\theta = 0$ . Figs. 1b and c reveal that such minima in  $v_x/\theta$  relationships do not occur for  $\theta = 0$  or  $\pm\theta_p$ , whereas a minimum does occur at  $\theta = 0$  in the  $v_y/\theta$  relationship, but not at  $\theta = \pm\theta_p$ . Other minima in these relationships do not correspond to  $\theta$  values which have any potential for forming equilibrium profiles. However, if one generalizes the requirement for stability, that the total wave velocity, given by  $v^2 = v_x^2 + v_y^2$ , should be minimized with respect to angle  $\theta$ , then an important result emerges. The total velocity,  $v$ , is plotted in Fig. 1d, as a function of  $\theta$ , where it is noted that a minimum occurs at  $\theta = 0$ , a maximum at  $\theta = \pm\theta^*$ , and points of inflection at  $\theta = \pm\theta_{S_1}, \pm\theta_{S_2}$ . The angles  $\pm\theta_p$  do not correspond to any of these points and indeed lie in the range  $\theta^* < \theta_p < \theta_{S_2}$ . The behaviour of this  $v/\theta$  function, as described above, is readily proved by noting that differentiation of the defining equation for  $v$ ,

$$v = \frac{\Phi}{N} \left[ \left( \frac{dS}{d\theta} \cos \theta \right)^2 + \left( \frac{dS}{d\theta} \sin \theta \cos \theta - S \right)^2 \right]^{1/2}$$

with respect to  $\theta$ , leads to a minimum or maximum where  $(dS/d\theta)\cos\theta - S\sin\theta = 0$  which is satisfied as a minimum when  $\theta = 0$  and a maximum when  $(dS/d\theta)_{\theta^*} = S_{\theta^*} \cdot \tan\theta^*$ , and points of inflection at  $\pm\theta_{S_1}, \pm\theta_{S_2}$  which satisfy

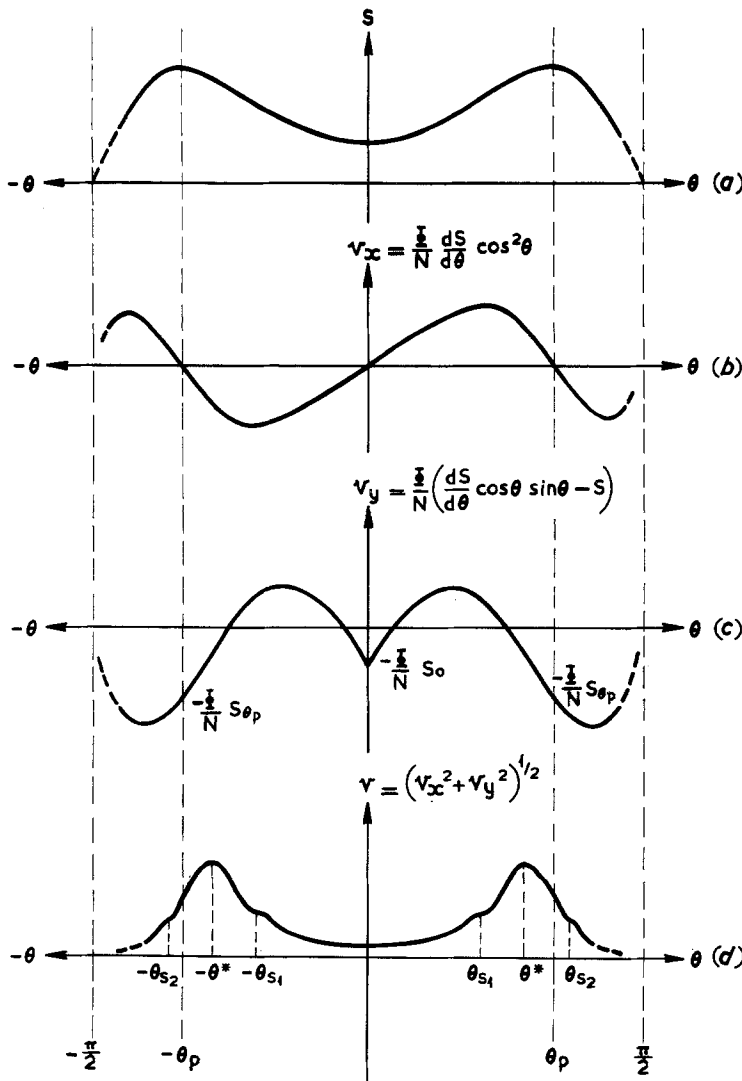


Figure 1 Schematic representation of the behaviour of parameters  $S$ ;

$$v_x = \frac{\Phi}{N} \frac{dS}{d\theta} \cos^2 \theta$$

$$v_y = \frac{\Phi}{N} \left( \frac{dS}{d\theta} \cos \theta \sin \theta - S \right)$$

and  $v = (v_x^2 + v_y^2)^{1/2}$  as functions of angle  $\theta$

$(d^2S/d\theta^2)\cos \theta - 2(dS/d\theta)\sin \theta = 0$ . It is interesting to note that these values of  $\theta_{S_1}$ ,  $\theta_{S_2}$  correspond to points of inflection [3] on the erosion slowness curve [7] which plots the parameter  $S_0/(S \cos \theta)$  as a function of  $\theta$  and to extrema in the curve  $v_x$  as a function of  $v_y$  [1].

It therefore appears that *only* the  $\theta = 0$  configuration satisfies the equilibrium requirements that  $v_x = \text{constant}$  ( $= 0$ ) and  $v_y = \text{constant}$  ( $= -S_0$ ) and the stability requirement that  $dv/d\theta = 0$ . Thus the flat surface, normal to the ion flux, is most stable against perturbation, although the  $\theta = \pm \theta_p$  configuration may be regarded as a metastable state, but that significant perturbations in  $\theta$  (e.g. a surface discontinuity or inhomogeneity) may result in driving this state, eventually to the

flat surface. It will be interesting to conduct experimental studies to determine the long term stability of the "cone forests" which have been observed [6] as a feature within a bounded surface grain on Cu.

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### *Determination of the recovery stresses developed by shape memory alloys*

The mechanical shape memory effect is exhibited by several alloys, all of which undergo thermoelastic martensitic transformation [1]. The memory effect is demonstrated by inducing a macroscopic strain within a certain range in a specimen while in the martensitic state, and then heating to revert martensite to the high temperature phase (HTP). During reversion, the specimen tends to recover its original unstrained shape. Strain recovery starts at the  $A_s$  temperature and finishes at the  $A_f$  temperature\*.

One of the most interesting applications of shape memory alloys is in energy conversion devices that utilize the memory effect in converting low grade heat sources into useful mechanical work [2–4]. In evaluating the performance of a particular alloy in such devices it becomes essential to determine the levels of recovery stresses† developed during the martensite → HTP transformation upon heating. There have been a few investigations dealing with experimental measurements of the recovery stresses developed by Ni–Ti alloy near the equi-atomic composition [5, 6]. However, no attempt has been made as yet to predict these stresses. In the present paper, a simple relationship has been developed between the recovery stresses, temperature and strain.

For the discussions which follow, it is instructive to identify a reference point from which the macroscopic strain is measured i.e., a zero-point strain. This can conveniently be taken to be the point at which the material consists entirely of the HTP.

\*  $A_s$  = temperature at which the martensite → HTP transformation starts during heating.

$A_f$  = temperature at which this transformation finishes during heating.

† A recovery stress is defined as the external stress required to balance the internal stresses that tend to revert martensite to the HTP.

Consider a polycrystalline shape memory alloy that has been almost entirely transformed to martensite by cooling it to a temperature at or below its respective martensite finish temperature  $M_f$ . In the absence of an external or appreciable internal stresses, all the martensite variants that are crystallographically equivalent would form with equal probability. Therefore, no net macroscopic strain as measured from the zero-point would be expected, and hence no recovery stresses would develop during the reverse transformation to the HTP. In order to realize a recovery stress, the material must acquire a macroscopic strain relative to the zero-point. In terms of the microstructural features, this corresponds to a certain degree of directionality in the distribution of the martensite variants throughout the microstructure. It has been shown experimentally that any strain within the recoverable range is accommodated by reorientation of a volume fraction of the thermally induced martensite [7–10]. This occurs by preferential growth of the most favourably oriented martensite variants. It is then expected that the recovery stress,  $\sigma_r$ , would be proportional to the volume fraction of re-oriented martensite ( $V_M$ ). This determines the functional dependence of  $\sigma_r$ , on strain  $\epsilon$ .

Upon heating to within the  $A_s$ – $A_f$  temperature range a certain volume fraction of martensite tends to revert to the HTP. The driving force for such reversion arises from the chemical free energy difference between the two respective structures, the elastic strain energy stored in the lattice during the transformation to martensite and energy associated with reversible defects, e.g., twins. As the temperature increases within the range  $A_s$ – $A_f$ ,