Slip-Induced Directional Order Theory for $B2$-Type Superlattices

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SUMMARY

The theory of slip-induced directional order has been developed for the B2*-type superlattices. The treatment is based on the original work of Chikazumi* et al. *Separate analyses have been made for slip on* {110} ⟨111⟩ *and* {112} ⟨111⟩ *systems, which are prominent slip systems in b.c.c. alloys. In addition, consideration has been made for both long- and short-range order in the structure, as well as for nearest-neighbor and next-nearest-neighbor interactions.*

The results of the analysis are summarized as follows: (1) *In the case of nearest-neighbor interactions,* (a) {110} ⟨111⟩ *slip in both long- and short-range ordered lattices results in the slip plane normal as the effective direction of excess* like-atom *pairs*; (b) {112} ⟨111⟩ *slip, on the other hand, results in the slip direction as the effective direction of* unlike *pairs.* (2) *In the case of next-nearest-neighbor interactions,* (a) {110} ⟨111⟩ *slip in both long- and short-range ordered lattices leads to that* ⟨100⟩ *direction which lies on the slip plane, as the effective like-pair direction, while* (b) *no anisotropy is expected from slip in* {112} ⟨111⟩ *systems.*

The theory is applied to FeCo, whereby the magnetic anisotropy energy obtained by rolling single crystals of (001)[$\bar{1}$10], (115)[$\bar{1}$10], (112)[$\bar{1}$10], (111) [$\bar{1}$10] *and* (110) [$\bar{1}$10] *orientations are calculated. Except for* (110) [$\bar{1}$10], *these orientations comprise the crystallographic texture spread as found in heavily rolled polycrystalline material near the FeCo composition. The results of the calculations are in good agreement with the observations of Fahlenbrach* et al. *if mixed slip of both* {110}⟨111⟩ *and* {112}⟨111⟩ *slip systems (pencil glide) is assumed to take place during deformation. Such mixed slip has been observed by Stoloff and Davies.*

Possible contributions from magnetocrystalline and magnetostrictive anisotropies to the observed results of rolled FeCo are also discussed.

RÉSUMÉ

L'auteur a élaboré une théorie de l'ordre directionnel créé par la déformation par glissement dans les surstructures de type B2. *Son calcul repose sur le modèle théorique proposé initialement par Chikazumi* et al. *Il a analysé séparément les cas où le glissement actif est* {110}⟨111⟩ *et* {112}⟨111⟩; *ces deux systèmes sont en effet les systèmes de glissement prédominants dans les alliages de structure cubique centrée. De plus il a considéré à la fois les situations où la structure possédait un ordre à grande distance et celles où elle était caractérisée par un ordre à courte distance et il a fait intervenir aussi bien les interactions entre premier voisins que celles entre seconds voisins.*

Les résultats de cette analyse peuvent être résumés de la manière suivante: (1) *Si l'on considère seulement les interactions entre premiers voisins,* (*a*) *le glissement du système* {110}⟨111⟩ *aboutit à la création dans les structures ordonnées d'un excédent de* paires d'atomes semblables *dans la direction perpendiculaire au plan de glissement, que l'ordre soit à grande distance ou à courte distance*; (*b*) *par contre le glissement du système* {112}⟨111⟩ *aboutit à la formation d'un excédent de* paires d'atomes dissemblables *dans la direction de glissement.* (2) *Si l'on tient compte des interactions entre seconds voisins,* (*a*) *le glissement* {110} ⟨111⟩ *conduit à un excédent de paires d'atomes semblables dans celle des directions* ⟨100⟩ *qui est contenue dans le plan de glissement, dans le cas de l'ordre à grande distance aussi bien que dans celui de l'ordre à courte distance, tandis que* (*b*) *on ne doit s'attendre à*

and $[1\bar{1}1]$) that lie on the (110) slip plane, we still have four AB pairs each. On the other hand, along $[\bar{1}\bar{1}1]$ and [111], which lie on the $(1\bar{1}0)$ plane, we now have two AA pairs and two BB pairs. Hence, we gain two BB pairs each along $[\bar{1}\bar{1}1]$ and [111]. If there is partial ordering, as expressed by the LRO parameter s, $\Delta N_{BB}=2s^2$ (see Appendix). Since the area of (110) planes in Fig. 1 is $2a^2\sqrt{2}$, we have $\Delta N_{BB}=s^2/a^2\sqrt{2}$ per unit (110) area. In addition, as discussed by Chikazumi *et al.*[1], this quantity is obtained by assuming that an *odd* number of *unit* dislocations have passed on each *slipped* plane. Thus, we insert a factor of $\frac{1}{2}$ for the chance that an odd number of dislocations had passed, and a factor p_0 for the probability that a unit dislocation is not paired with another to form a superdislocation, as it tends to do when long-range order is present. Finally, the number of slip planes (per unit distance perpendicular to the slip plane) that have *slipped* is equal to $|\gamma|/nb$ where γ is the macroscopic glide-shear resulting from the slip, n is the average number of dislocations passed per *slipped* plane, and $b=a\sqrt{3}/2$ is the Burger's vector. Thus, per unit volume,

$$\Delta N_{BB}=\frac{p_0}{2}\frac{s^2}{a^2\sqrt{2}}\frac{|\gamma|}{nb}=\frac{Np_0s^2|\gamma|}{2\sqrt{6n}}, \qquad (2)$$

where $N=2/a^3$ is the number of atoms per unit volume. Equation (2) can be converted to Chikazumi's notation by letting $p'=1/n$ as the probability of passing a dislocation per atomic (slip) plane, and noting that $\gamma=Sb/d$ where S is the "slip density", or the average (effective) number of dislocations passed per atomic (slip) plane, and $d=a/\sqrt{2}$ is the slip plane spacing. Then eqn. (2) becomes

$$\Delta N_{BB}=\tfrac{1}{4}Np_0p's^2S. \qquad (3)$$

Since the directions of the BB pairs thus induced by (110) $[\bar{1}11]$ slip are $[\bar{1}\bar{1}1]$ and [111], eqn. (1) becomes

$$E=\tfrac{1}{4}Nlp_0p's^2S\left[\left(-\frac{1}{\sqrt{3}}\alpha_1-\frac{1}{\sqrt{3}}\alpha_2+\frac{1}{\sqrt{3}}\alpha_3\right)^2+\left(\frac{1}{\sqrt{3}}\alpha_1+\frac{1}{\sqrt{3}}\alpha_2+\frac{1}{\sqrt{3}}\alpha_3\right)^2\right]=$$
$$=\tfrac{1}{3}Nlp_0p's^2S(\alpha_1\alpha_2)+\text{const}, \qquad (4)$$

where α_1, α_2, α_3 are the direction cosines of the local magnetization vector with respect to the cubic axes. The functional dependence $\alpha_1\alpha_2$ in eqn. (4) means that the slip plane normal [110] is the effective BB pair direction. (It may also be deduced from the fact that [110] is symmetrically disposed (at an angle $<45°$) with respect to $[\bar{1}\bar{1}1]$ and [111].) Hence, in accordance with the assumption $Nl<0$, the slip plane normal becomes an easy axis of magnetization as a result of slip.

In the general case where n_{1i}, n_{2i}, n_{3i} are the direction cosines of the slip plane normal of the ith system, we have

$$E=\tfrac{2}{3}Nlp_0p's^2\sum_i|S_i|(n_{1i}n_{2i}\alpha_1\alpha_2+n_{2i}n_{3i}\alpha_2\alpha_3+n_{3i}n_{1i}\alpha_3\alpha_1), \qquad (5)$$

where the summation is carried over all active slip systems i.

For the case of short range order, the directions of BB pairs induced by $(110)[\bar{1}11]$ slip are again $[\bar{1}\bar{1}1]$ and [111]. It turns out that in the two unit cells of Fig. 1a, the number of BB pairs in each $\langle 111\rangle$ direction before slip is $1-\sigma$, where σ is the Bethe short-range order parameter (see Appendix). According to Cohen and Fine[12], the structure across the slip planes becomes random after three or four slip steps. Hence we may take $\sigma=0$ after slip, so that the number of BB pairs gained by slip is $\sqrt{2}\sigma/4a^2$ per unit (110) area. To this we multiply by $|\gamma|/nb$, the effective number of *slipped* planes (per unit distance perpendicular to the slip plane). Thus

$$\Delta N_{BB}=\frac{\sqrt{2}\sigma|\gamma|}{4na^2b}=\tfrac{1}{4}Np'\sigma S, \qquad (6)$$

with the direction cosines of the BB pairs the same as the LRO case. By combining eqns. (5) and (6), we finally obtain the induced uniaxial anisotropy energy

$$E_{NN}=\tfrac{2}{3}E_1\sum_i|S_i|(n_{1i}n_{2i}\alpha_1\alpha_2+n_{2i}n_{3i}\alpha_2\alpha_3+n_{3i}n_{1i}\alpha_3\alpha_1), \qquad (7)$$

where $E_1\equiv Nlp'(p_0s^2+\sigma)$, and the subscript NN denotes the nearest neighbor case.

(*b*) *Next-nearest-neighbor (NNN) interactions*

In the body-centered cubic structure, the distance between next nearest neighbors is only 13.5% greater than that between nearest neighbors; hence NNN interactions may become important, especially in certain symmetric orientations where NN contributions to the slip-induced anisotropy become small.