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THE INTERFACIAL TENSION OF A SHARP ANTIPHASE DOMAIN BOUNDARY

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ABSTRACT

The central result of this paper is an analytic solution for the interfacial tension of a sharp antiphase boundary in an ordered binary crystal whose atoms interact in pairs. The general solution is valid for an arbitrarily long-range interatomic interaction, and for any orientation of the antiphase boundary in any superstructure. The result can be expressed in terms of the Fourier transform of the interaction energy, V(k), or may alternately be written as a series in the potentials, W_i, that govern the interaction between solutes in the ith nearest neighbor positions. In the latter case the coefficients of the successive terms in the series are integrals of simple trigonometric expressions. The results are specified to treat {111} and {100} antiphase boundaries in the $L1_2$ (Cu_3Au-type) structure and {100} boundaries in the $L1_0$ (CuAuI-type) structure. The equations are exhibited for interactions up to the eighth nearest neighbors. The tension of the {111} antiphase boundary in the Al_3Li ($L1_2$) phase is computed in a second-neighbor interaction model in which the interatomic potentials are chosen to give a best fit to the phase diagram. The result, 72 erg/cm^2, is in reasonable agreement with the most recent determinations by other techniques.

I. INTRODUCTION

An antiphase domain boundary separates two regions of ordered crystal that differ from one another by a translation along a basis vector of the superlattice unit cell. Since the structures are otherwise identical, the increase in energy when an antiphase domain is introduced into a stable ordered crystal can be attributed to the antiphase boundary itself and associated with the interfacial tension of the

boundary, σ^A.

In a model solid whose atoms interact only with their nearest neighbors the antiphase boundary energy can be computed from the change in the numbers and types of nearest neighbors that is caused by the antiphase shift. Such calculations were done by Flinn [1960] for antiphase boundaries with 1/2<110> displacement vectors in the $L1_2$ structure.

However, the nearest-neighbor bonding model is always an oversimplification, and specifically cannot apply to the $L1_2$ structure since interactions with more distant neighbors are required to stabilize the structure in its long-range ordered state [Danielian, 1961, 1969]. More generally, in any ordered intermetallic structure there is a resonance between the conduction electrons at the Fermi surface and the ordering concentration waves that automatically introduces a long-range effective interaction [Krivoglaz, 1983]. Recent developments in the electron theory of metals make it possible to determine the long-range interaction in ordered systems [for example, Stocks, et al., 1986].

Several researchers have incorporated some of this behavior into treatments of antiphase boundaries. Krasko [1969] expressed the antiphase boundary energy of the $L1_2$ structure in terms of the equilibrium short-range order parameters of the relevant disordered alloy; Foiles [1986] used the "embedded atom" method to calculate the equilibrium configuration and energy of the {111} and {100} antiphase boundaries in γ' Ni_3Al, which has the $L1_2$ structure; Sanchez, et al. [1986] used a short range interaction along with a cluster variation technique to study the same boundaries. The latter methods are, however, specific to a given boundary and set of experimental conditions. It remains desirable to find a general analytic technique for estimating the tension of an antiphase boundary with arbitrary orientation in an arbitrary ordered structure while accounting for long-range interactions.

If we confine our attention to sharp boundaries in systems whose atoms interact in pairs, we might attempt the problem by generalizing the method of Flinn [1960] to include interactions with more distant neighbors. This approach is made difficult by the problem of counting the number of pairs that are changed by an antiphase displacement. In fact, if the method is extended beyond the immediate neighbors the counting problem alone would seem to require a specific computer solution for each individual case. We have, therefore, taken an alternate approach which is both completely general and relatively straightforward.

Since the energy associated with the introduction of an antiphase domain can be wholly attributed to its boundaries, a theory that calculates the energy of an arbitrary distribution of antiphase domains can be used to compute the tension of an antiphase boundary in any orientation. We need only let the antiphase domain be a plate that is extended along the habit plane of interest; the total energy of the domain is twice the boundary energy. When the atoms interact in pairs such a theory can be constructed without imposing any restriction on the range of interatomic interaction by applying the method of concentration waves [Khachaturyan, 1962, 1973, 1978].

The theory is developed in four parts. In the first we describe the atomic distribution in an ordered binary crystal that contains an arbitrary distribution of antiphase domains. In the second we calculate the free energy increment due to the antiphase domains. In the third we specialize the result to the case of an extended antiphase domain along a particular crystallographic plane, and obtain a general analytic solution for the tension of an antiphase boundary. In the fourth we apply this solution to three cases of particular interest: {111} and {100} boundaries in the $L1_2$ (Cu_3Au) structure, which are the important antiphase boundaries in the γ' Ni_3Al and δ' Al_3Li phases, among others, and {100} boundaries in the $L1_0$ (CuAuI) structure.

The specific development that is given here assumes a sharp antiphase boundary in an ordered binary solution of atoms distributed over the sites of a rigid lattice. It hence neglects any elastic distortion or atomic redistribution that may occur near the boundary. Since any equilibrium relaxation decreases the interfacial tension, the computed value is an upper bound. However, the result should be accurate for antiphase boundaries that form at low temperature, and is specifically applicable to the important case of an antiphase boundary created by the passage of a partial dislocation during plastic deformation at moderate temperature.

II. THE SOLUTE DISTRIBUTION IN AN ORDERED BINARY SOLUTION WITH ANTIPHASE DOMAINS

A. The Solute Distribution

The solute distribution in a binary crystal is specified by a function, $x(r)$, defined at the lattice sites, r, of the fully disordered parent structure, that gives the probability that an atom of a particu-

lar type (the "solute") will be found at the site, $\mathbf{r}$. If the solution has a high degree of long-range order and a nearly stoichiometric composition the variable, $x(\mathbf{r})$, has a value very close to either 0 or 1 at every lattice site.

Let the ordered crystal contain an arbitrary distribution of antiphase domains, and let $\mathbf{b}_\alpha$ be the vector that gives the antiphase shift in the αth domain. The antiphase vector, $\mathbf{b}_\alpha$, is always a translation vector of the disordered parent lattice but, by definition, is not a translation vector of the ordered superlattice. It follows that the number of possible values of $\mathbf{b}_\alpha$ is equal to the number of lattice sites within the smallest unit cell of the superlattice.

If $x^\circ(\mathbf{r})$ is the solute distribution within a reference domain of the ordered crystal the distribution within the αth domain can be written

$$x_\alpha(\mathbf{r}) = x^\circ(\mathbf{r}+\mathbf{b}_\alpha) \tag{1}$$

Moreover, the shape of the αth domain can be specified by the function, $\theta_\alpha(\mathbf{r})$, which has the value

$$\begin{aligned} \theta_\alpha(\mathbf{r}) &= 1 \qquad &&(\mathbf{r} \text{ in the } \alpha\text{th domain}) \\ &= 0 \qquad &&(\text{otherwise}) \end{aligned} \tag{2}$$

With this notation the solute distribution is

$$x(\mathbf{r}) = \Sigma_\alpha x^\circ(\mathbf{r}+\mathbf{b}_\alpha)\theta_\alpha(\mathbf{r}) \tag{3}$$

The solute distribution can always be written as a sum of concentration waves [Khachaturyan, 1963, 1973, 1978]:

$$x(\mathbf{r}) = (1/N^\circ)\Sigma_\mathbf{k} x(\mathbf{k})e^{i\mathbf{k}\mathbf{r}} \tag{4}$$

where N° is the total number of crystal lattice sites, $x(\mathbf{k})$ is the amplitude of the concentration wave with wave vector $\mathbf{k}$, $\mathbf{k}\mathbf{r}$ is the scalar product between the vectors $\mathbf{k}$ and $\mathbf{r}$, and the sum is taken over the N° wave vectors, $\mathbf{k}$, in the first Brillouin zone of the disordered parent structure, whose values are determined by cyclic boundary conditions on the whole crystal. The amplitudes of the solute concentration waves, $x(\mathbf{k})$, are the Fourier transforms

$$x(\mathbf{k}) = \Sigma_\mathbf{r} x(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}} \tag{5}$$

B. Concentration Waves in the Presence of Antiphase Domains

We wish to describe the solute distribution in an ordered crystal that contains an arbitrary distribution of antiphase domains. Using equation (3), the concentration wave amplitudes are

$$\begin{aligned} x(k) &= \Sigma_r e^{-ikr}\{\Sigma_\alpha x^\circ(r+b_\alpha)\theta_\alpha(r)\} \\ &= (N^\circ)^{-1}\Sigma_{k'}\Sigma_\alpha x^\circ(k',b_\alpha)\theta_\alpha(k-k') \end{aligned} \tag{6}$$

where

$$x^\circ(k',b_\alpha) = \Sigma_r x^\circ(r+b_\alpha)e^{-ik'r} \tag{7}$$

$$\theta_\alpha(k-k') = \Sigma_r \theta(r)e^{-i(k-k')r} \tag{8}$$

The solute distribution in a homogeneously ordered crystal can always be written [Khachaturyan, 1962, 1978]

$$x^\circ(r) = \bar{x} + \Sigma_j \gamma_j e^{ik_j r} \tag{9}$$

where $\bar{x}$ is the average concentration of the solute and the k_j are the wave vectors of the concentration waves that generate the superstructure. The solute distribution within the αth antiphase domain is, then,

$$x^\circ(r+b_\alpha) = \bar{x} + \Sigma_j \gamma_j \exp(ik_j b_\alpha)\exp(ik_j r) \tag{10}$$

The amplitude of the kth concentration wave associated with this distribution is

$$\begin{aligned} x^\circ(k,b_\alpha) &= \Sigma_r x^\circ(r+b_\alpha)e^{-ikr} \\ &= N^\circ[\bar{x}\delta(k) + \Sigma_j \gamma_j \exp(ik_j b_\alpha)\delta(k-k_j)] \end{aligned} \tag{11}$$

where $\delta(k)$ is equal to unity when $k=0$ and is zero otherwise. The amplitude of the kth concentration wave in a crystal that contains an arbitrary distribution of antiphase domains is found by substituting equation (11) into equation (6):

$$\begin{aligned} x(\mathbf{k}) &= \Sigma_\alpha[\bar{x}\theta_\alpha(\mathbf{k}) + \Sigma_j\gamma_j\exp(i\mathbf{k}\mathbf{b}_\alpha)\theta_\alpha(\mathbf{k}-\mathbf{k}_j)] \\ &= x^o(\mathbf{k}) + \Sigma_{j,\alpha}\{\gamma_j[e^{(i\mathbf{k}_j\mathbf{b}_\alpha)}-1]\theta_\alpha(\mathbf{k}-\mathbf{k}_j)\} \\ &= x^o(\mathbf{k}) + \Delta x^A(\mathbf{k}) \end{aligned} \tag{12}$$

In this equation,

$$\begin{aligned} x^o(\mathbf{k}) &= \bar{x}\Sigma_\alpha\theta_\alpha(\mathbf{k}) + \Sigma_j\gamma_j[\Sigma_\alpha\theta_\alpha(\mathbf{k}-\mathbf{k}_j)] \\ &= N^o[\bar{x}\delta(\mathbf{k}) + \Sigma_j\gamma_j\delta(\mathbf{k}-\mathbf{k}_j)] \end{aligned} \tag{13}$$

where we have used the identity,

$$\begin{aligned} \Sigma_\alpha\theta_\alpha(\mathbf{k}) &= \Sigma_\mathbf{r}e^{-i\mathbf{k}\mathbf{r}}[\Sigma_\alpha\theta_\alpha(\mathbf{r})] = \Sigma_\mathbf{r}e^{-i\mathbf{k}\mathbf{r}} \\ &= N^o\delta(\mathbf{k}) \end{aligned} \tag{14}$$

The $x^o(\mathbf{k})$ are the Fourier amplitudes of the concentration waves in the homogeneous reference state. The $\Delta x^A(\mathbf{k})$ are the amplitudes of the concentration waves that perturb the homogeneous concentration field when the antiphase domains are introduced, and are

$$\Delta x^A(\mathbf{k}) = \Sigma_{j,\alpha}\{\gamma_j[e^{(i\mathbf{k}_j\mathbf{b}_\alpha)}-1]\theta_\alpha(\mathbf{k}-\mathbf{k}_j)\} \tag{15}$$

III. THE ENERGY OF AN ARBITRARY DISTRIBUTION OF ANTIPHASE DOMAINS

If the states of a binary solution are distributions of atoms over a fixed lattice then the equilibrium of the solution is controlled by its Helmholtz free energy, F. When, moreover, the solution is nearly stoichiometric and the long-range order parameter is high, F can be evaluated in the mean field approximation. We need only consider that part of the Helmholtz free energy, F^c, that depends on the solute configuration. Assuming that the atoms interact in pairs, the configurational part of the free energy is given in terms of the concentration field by [Khachaturyan, 1978]

$$\begin{aligned} F^c = {} & (1/2)\Sigma_{\mathbf{r},\mathbf{r}'}W(\mathbf{r}-\mathbf{r}')x(\mathbf{r})x(\mathbf{r}') \\ & + kT\Sigma_\mathbf{r}\{x(\mathbf{r})\ln[x(\mathbf{r})]+[1-x(\mathbf{r})]\ln[1-x(\mathbf{r})]\} \end{aligned} \tag{16}$$

where $W(\mathbf{r}-\mathbf{r}')$ is the interchange interaction energy between solute atoms on sites at $\mathbf{r}$ and $\mathbf{r}'$, T is the absolute temperature and k is Boltzmann's

constant.

If we neglect relaxations near the antiphase boundaries the configurational entropy of the solution is negligibly changed by the introduction of antiphase boundaries. It follows that the relevant part of the free energy is the configurational energy

$$\begin{aligned} E^c &= (1/2)\Sigma_{r,r'}W(r-r')x(r)x(r') \\ &= (1/2N^o)\Sigma_k V(k)|x(k)|^2 \end{aligned} \tag{17}$$

where the second form is obtained by taking the Fourier transform and the interaction potential, $V(k)$, is

$$V(k) = \Sigma_r W(r)e^{-ikr} \tag{18}$$

The configurational energy of an ordered phase that contains an arbitrary distribution of antiphase domains is obtained by substituting the composition amplitudes, equation (12), into (18). The result is

$$\begin{aligned} E^c &= (1/2N^o)\Sigma_k V(k)[x^o(k) + \Delta x^A(k)][x^o(k) + \Delta x^A(k)]^* \\ &= (1/2N^o)\Sigma_k V(k)|x^o(k)|^2 \\ &\quad + (1/2N^o)\Sigma_k V(k)[x^o(k)\Delta x^A(k)^* + x^o(k)^*\Delta x^A(k)] \\ &\quad + (1/2N^o)\Sigma_k V(k)|\Delta x^A(k)|^2 \end{aligned} \tag{19}$$

The first term on the right in equation (19) is the energy of a homogeneously ordered phase. The second two terms give the increment to the configurational energy due to the antiphase domains. It follows with the help of equations (13) and (15) that

$$\begin{aligned} \Delta E^A = (1/2N^o)\Sigma_k\Sigma_{jm\alpha\beta}\{V(k)\gamma_j\gamma_m^*[e^{i(k_j b_\alpha)}-1][e^{-i(k_m b_\beta)}-1]\theta_\alpha(k-k_j)\theta_\beta^*(k-k_m)\} \\ + (1/2)\Sigma_k\Sigma_{j\alpha}V(k)\{\gamma_j[e^{i(k_j b_\alpha)}-1]\theta_\alpha(k-k_j)[\bar{x}\delta(k)+\Sigma_m\gamma_m^*\delta(k-k_m)] \\ + \gamma_j^*[e^{-i(k_j b_\alpha)}-1]\theta_\alpha^*(k-k_j)[\bar{x}\delta(k)+\Sigma_m\gamma_m^*\delta(k-k_m)]\} \end{aligned} \tag{20}$$

Equation (20) can be simplified substantially by using the properties of the Fourier transform, $\theta(k)$, of the shape function of an antiphase domain. It follows from its definition (equation (8)) that this functions vanishes when $|k|$ is greater than $\sim 2\pi/L$, where L is the dimension of the antiphase domain in the direction of k. But the wave

vectors $\mathbf{k}_j$ and $\mathbf{k}_j-\mathbf{k}_m$ $(j \neq m)$ are of the order $2\pi/a_s$, where a_s is the lattice parameter of the superlattice. Hence when the antiphase domain is large compared to the crystal lattice parameter, which is the case that interests us, the Fourier transforms $\theta_\alpha(\mathbf{k}_j)$ can be neglected, and the transforms $\theta_\alpha(\mathbf{k}_m-\mathbf{k}_j)$ and $\theta_\alpha(\mathbf{k}-\mathbf{k}_j)\theta^*_\beta(\mathbf{k}-\mathbf{k}_m)$ can also be neglected unless j=m. It follows that we may set j=m in equation (20), which simplifies to

$$\begin{aligned}\Delta E^A &= (1/2N^\circ)\Sigma_{\mathbf{k}}\Sigma_{j\alpha\beta}\{V(\mathbf{k})|\gamma_j|^2[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}-1][e^{-i(\mathbf{k}_j\mathbf{b}_\beta)}-1]\theta_\alpha(\mathbf{k}-\mathbf{k}_j)\theta^*_\beta(\mathbf{k}-\mathbf{k}_j)\} \\ &\quad + (1/2)\Sigma_{j\alpha}\{V(\mathbf{k}_j)|\gamma_j|^2\theta_\alpha(0)[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}+e^{-i(\mathbf{k}_j\mathbf{b}_\alpha)}-2]\} \qquad (21) \\ &= (1/2N^\circ)\Sigma_{\boldsymbol{\kappa}}\Sigma_{j\alpha\beta}\{V(\mathbf{k}_j+\boldsymbol{\kappa})|\gamma_j|^2[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}-1][e^{-i(\mathbf{k}_j\mathbf{b}_\beta)}-1]\theta(\boldsymbol{\kappa})\theta^*_\beta(\boldsymbol{\kappa})\} \\ &\quad + (1/2)\Sigma_{j\alpha}\{V(\mathbf{k}_j)|\gamma_j|^2\theta_\alpha(0)[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}+e^{-i(\mathbf{k}_j\mathbf{b}_\alpha)}-2]\}\end{aligned}$$

where we have used the vector $\boldsymbol{\kappa}$,

$$\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}_j \qquad (22)$$

The second term in equation (21) can be cast into the same form as the first if we use the identity

$$\begin{aligned}(1/N^\circ)\Sigma_{\boldsymbol{\kappa}}\theta_\alpha(\boldsymbol{\kappa})\theta^*_\beta(\boldsymbol{\kappa}) &= N^\alpha\delta_{\alpha\beta} = [\Sigma_\alpha\theta_\alpha(\mathbf{r})]\delta_{\alpha\beta} \\ &= \theta_\alpha(0)\delta_{\alpha\beta}\end{aligned} \qquad (23)$$

where N^α is the number of lattice sites in the αth domain. Then

$$\begin{aligned}&\theta_\alpha(0)[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}+e^{-i(\mathbf{k}_j\mathbf{b}_\alpha)}-2] = \\ &\qquad - [e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}-1][e^{-i(\mathbf{k}_j\mathbf{b}_\beta)}-1](1/N^\circ)\Sigma_{\boldsymbol{\kappa}}\theta_\alpha(\boldsymbol{\kappa})\theta^*_\beta(\boldsymbol{\kappa})\end{aligned} \qquad (24)$$

and equation (21) can be rewritten

$$\Delta E^A = (1/2N^\circ)\Sigma_j\{|\gamma_j|^2\Sigma_{\boldsymbol{\kappa}}[V(\mathbf{k}_j+\boldsymbol{\kappa})-V(\mathbf{k}_j)]|\Omega(\mathbf{k}_j,\boldsymbol{\kappa})|^2\} \qquad (25)$$

where

$$|\Omega(\mathbf{k}_j,\boldsymbol{\kappa})|^2 = \Sigma_{\alpha\beta}[e^{i(\mathbf{k}_j\mathbf{b}_\alpha)}-1][e^{-i(\mathbf{k}_j\mathbf{b}_\beta)}-1]\theta_\alpha(\boldsymbol{\kappa})\theta^*_\beta(\boldsymbol{\kappa}) \qquad (26)$$

Equation (25) is the solution for the excess energy associated with an arbitrary distribution of antiphase domains.

III. THE TENSION OF AN ANTIPHASE DOMAIN BOUNDARY ON THE (hkl) PLANE

A. The Tension of a Single Antiphase Domain Boundary

Since the antiphase domains have identical structures the excess energy of a collection of antiphase domains can be wholly attributed to the domain boundaries. If the boundaries are sharp, that is, if relaxations in the vicinity of the boundary can be neglected, the excess energy is simply the integral of the interfacial tension over the antiphase boundary area:

$$\Delta E^A = \int_S \sigma^A(\mathbf{m})dS \tag{27}$$

where $\sigma^A(\mathbf{m})$ is the tension of an element of antiphase boundary (dS) with the normal vector, $\mathbf{m}$, and the integral is taken over the whole area of antiphase boundary.

Now let there be only one domain, and let it have the form of a flat plate on the plane (hkl). If the lateral extension of the plate, L, is large compared to its thickness, D, (small aspect ratio) then its lateral boundaries make a negligible contribution to the excess energy and

$$\Delta E^A = 2\sigma^A(hkl)S \tag{28}$$

where S is the surface area of the plane face of the plate. If, moreover, D is larger than the effective range of interatomic interaction, r^o, then $\sigma^A(hkl)$ is equal to the tension of an isolated boundary. The problem of computing the antiphase boundary energy is hence reduced to the problem of determining the excess energy due to an antiphase plate that has a thickness greater than the range of interatomic interaction ($r^o/D < 1$) but an extension large enough that its aspect ratio is small ($D/L \ll 1$).

If there is only a single antiphase domain the indices α and β and the summation can be eliminated from equation (26), which reduces to

$$\Omega(\mathbf{k}_j,\kappa) = [e^{i\mathbf{k}_j\mathbf{b}}-1]\theta(\kappa) \tag{29}$$

where $\theta(\kappa)$ is the Fourier transform of the shape function of the domain, and $\mathbf{b}$ is its antiphase vector. The excess energy is obtained by substituting equation (29) into (25), and is

$$\Delta E^A = 2N^s\Sigma_j|\gamma_j|^2\sin^2(k_jb/2)\Psi(k_j) \tag{30}$$

where N^s is the number of crystal lattice sites in the (hkl) plane that bounds the domain,

$$\Psi(k_j) = (1/N^sN^o)\Sigma_\kappa[V(\kappa+k_j)-V(k_j)]|\theta(\kappa)|^2 \tag{31}$$

and the relation $|e^{ik_jb}-1|^2 = 4\sin(k_jb/2)$ has been used. It follows that the tension of an antiphase boundary parallel to the (hkl) plane is

$$\begin{aligned}\sigma^A(hkl) &= (N^s/S)\Sigma_j|\gamma_j|^2\Psi(k_j)\sin^2(k_jb/2)] \\ &= (s)^{-1}\Sigma_j|\gamma_j|^2\Psi(k_j)\sin^2(k_jb/2)]\end{aligned} \tag{32}$$

where s is the area per atom in the (hkl) plane.

Of the parameters that appear on the right hand side of equation (32), the area per atom, s, is fixed by the parent structure and the indices, (hkl), of the boundary plane. The coefficients, γ_j, and the ordering wave vectors, k_j, are fixed by the structure of the ordered superlattice. Only the function $\Psi(k_j)$ needs to be evaluated.

B. The Function $\Psi(k_j)$

The function $\Psi(k_j)$ is evaluated by simplifying equation (31). We begin by evaluating the shape function, $\theta(\kappa)$. To facilitate this we define a new set of unit translations (A_1, A_2, A_3) for the disordered parent lattice, where A_1 and A_2 are chosen to lie in the (hkl) plane. Any reference vector of the disordered phase can then be written

$$\begin{aligned}r &= mA_1 + nA_2 + pA_3 \\ &= \rho + pA_3\end{aligned} \tag{33}$$

where m, n, p are arbitrary integers. The vector ρ lies in the (hkl) plane and enumerates the crystal lattice sites within the plane. The reciprocal vectors to the set A_i are defined by the relations

$$A_i^* = (A_j x A_k)/[A_i(A_j x A_k)] \qquad (i,j,k = 1,2,3) \tag{34}$$

An arbitrary wave vector, κ, in the first Brillouin zone of the disordered crystal can be written in terms of these:

$$\begin{aligned} \kappa &= 2\pi[\upsilon A_1^* + \mu A_2^* + \xi A_3^*] \\ &= \tau + 2\pi\xi A_3^* \end{aligned} \tag{35}$$

Using the orthogonality relations

$$A_i^* A_j = \delta_{ij} \tag{36}$$

the scalar product between κ and r is

$$\kappa r = (\tau+2\pi\xi A_3^*)(\rho+pA_3) = \tau\rho + 2\pi\xi p \tag{37}$$

The transformed shape function is then

$$\begin{aligned} \theta(\kappa) &= \Sigma_r \theta(r) e^{-i\kappa r} \\ &= [\Sigma_\rho e^{-i\tau\rho}][\Sigma_p e^{-i2\pi\xi p}] \\ &= \theta_s(\tau)\theta_3(\xi) \\ &= \theta_s(\tau)[e^{-i\pi\xi(N_z-1)}][\sin(\pi\xi N_z)/\sin(\pi\xi)] \end{aligned} \tag{38}$$

The second form of equation (38) shows that the shape function can be expressed as the product of two sums. The first defines the two-dimensional function, $\theta_s(\tau)$, by a summation over the sites on the (hkl) plane within the domain. The second sum defines the one-dimensional function, $\theta_3(\xi)$, and involves a summation over the (hkl) planes that lie within the domain. The function $\theta_3(\xi)$ is evaluated in the last form of equation (38). N_z is the number of (hkl) planes in the domain.

Given equation (38), the square of the shape function is

$$|\theta(\kappa)|^2 = |\theta_s(\tau)|^2[\sin^2(\pi\xi N_z)/\sin^2(\pi\xi)] \tag{39}$$

Substituting this result into equation (31) yields

$$\Psi(k_j) = (1/N^s N^o)\Sigma_\kappa[V(\kappa+k_j)-V(k_j)]|\theta_s(\tau)|^2[\sin^2(\pi\xi N_z)/\sin^2(\pi\xi)] \tag{40}$$

where $\kappa = \tau+2\pi\xi A^*_3$.

Equation (40) can be simplified further by using the properties of the shape function. The function $|\theta_s(\tau)|^2$ assumes non-vanishing values only within a range $|\Delta\tau| \sim 2\pi/L$ about $\tau = 0$, where L is the extension of the plate in the habit plane. Given its definition in

equation (18), the potential $V(\mathbf{k}+\tau)$ is equal to $V(\mathbf{k}) + O(r^0/L)$ when τ is confined to this range and r^0/L is small, and approaches the constant value $V(\mathbf{k})$ in the limit $(r^0/L) \to 0$. Hence when the extension of the plate in the habit plane is large compared to the range of interaction,

$$\begin{aligned} V(\mathbf{k}_j+\kappa)|\theta_s(\tau)|^2 &= V(\mathbf{k}_j+\tau+2\pi\xi\mathbf{A}_3^s)|\theta_s(\tau)|^2 \\ &\cong V(\mathbf{k}_j+2\pi\xi\mathbf{A}_3^s)|\theta_s(\tau)|^2 \end{aligned} \tag{41}$$

It follows that

$$\Psi(\mathbf{k}_j) = (1/N^sN^1)\Sigma_\xi[\Delta V(\mathbf{k}_j,\xi)][\sin^2(\pi\xi N_z)/\sin^2(\pi\xi)]\{(1/N^2)\Sigma_\tau|\theta_s(\tau)|^2\} \tag{42}$$

where $N^0 = N^1N^2$, N^1 is the total number of (hkl) planes in the crystal and N^2 is the number of the crystal lattice sites in an (hkl) plane that extends through the crystal, and

$$\Delta V(\mathbf{k}_j,\xi) = V(2\pi\xi\mathbf{A}_3^s+\mathbf{k}_j)-V(\mathbf{k}_j) \tag{43}$$

Since the function $|\theta_s(\tau)|^2$ obeys the identity

$$(1/N^2)\Sigma_\tau|\theta_s(\tau)|^2 = N^s \tag{44}$$

where N^s is the number of lattice sites in the portion of the (hkl) plane that lies within the domain,

$$\Psi(\mathbf{k}_j) = (1/N^1)\Sigma_\xi[\Delta V(\mathbf{k}_j,\xi)][\sin^2(\pi\xi N_z)/\sin^2(\pi\xi)] \tag{45}$$

The values of the variable ξ permitted by the cyclic boundary conditions are $\xi_n = (2\pi/N_1)n$, where n is an integer in the range $-N_1/2 \leq n \leq N_1/2$. Since N^1 is arbitrarily large the sum over ξ can be replaced by the integral

$$(1/N^1)\Sigma_\xi(\ldots) = \int_{-1/2}^{1/2} d\xi(\ldots) \tag{46}$$

so that

$$\Psi(\mathbf{k}_j) = \int_{-1/2}^{1/2} d\xi\{[\Delta V(\mathbf{k}_j,\xi)][\sin^2(\pi\xi N_z)/\sin^2(\pi\xi)]\} \tag{47}$$

Once $\Psi(\mathbf{k}_j)$ is evaluated from equation (47), the tension of the (hkl) antiphase boundary can be found by substituting the result into equation (32).

IV. APPLICATIONS TO FCC-BASED SUPERSTRUCTURES

To illustrate the calculation of the antiphase boundary tension we apply the general formalism to three cases of interest: the {111} and {100} boundaries in the $L1_2$ (Cu_3Au) structure, and the {100} boundary in the $L1_0$ (CuAuI) structure. In keeping with the way in which the problem is usually phrased we shall present the results as a series in the real-space interaction potentials, W_i, that give the interaction between a solute atom and neighboring solutes that are in the ith nearest shell. We shall also calculate one numerical example, the interfacial tension of the {111} antiphase boundary in δ' Al_3Li.

The Fourier transform, $V(\mathbf{k})$, of the interaction potential, $W(\mathbf{r})$, within a crystal can be expressed as a series in the interactions, W_i, with successively more distant neighbors. Writing the wave vector $\mathbf{k}$ in the form

$$\mathbf{k} = (2\pi/a)[\omega_1\mathbf{e}_1 + \omega_2\mathbf{e}_2 + \omega_3\mathbf{e}_3] \tag{48}$$

where the ω_i are the coordinates along three unit vectors, $\mathbf{e}_i$, parallel to the axes of the unit cell, the potential is

$$V(\mathbf{k}) = \Sigma_i V_i(\omega_1,\omega_2,\omega_3) \tag{49}$$

where V_i is the contribution from interaction with neighbors in the ith shell. The first eight terms in the series for the FCC structure are [Khachaturyan, 1963, 1978]

$$V_1 = 4W_1[\cos(\pi\omega_1)\cos(\pi\omega_2)+\cos(\pi\omega_2)\cos(\pi\omega_3)+\cos(\pi\omega_1)\cos(\pi\omega_3)] \tag{50}$$

$$V_2 = 2W_2[\cos(2\pi\omega_1)+\cos(2\pi\omega_2)+\cos(2\pi\omega_3] \tag{51}$$

$$\begin{aligned} V_3 = 8W_3[&\cos(2\pi\omega_1)\cos(\pi\omega_2)\cos(\pi\omega_3)+\cos(2\pi\omega_2)\cos(\pi\omega_1)\cos(\pi\omega_3) \\ &+ \cos(2\pi\omega_3)\cos(\pi\omega_1)\cos(\pi\omega_2)] \end{aligned} \tag{52}$$

$$\begin{aligned} V_4 = 4W_4[&\cos(2\pi\omega_1)\cos(2\pi\omega_2)+\cos(2\pi\omega_1)\cos(2\pi\omega_3) \\ &+ \cos(2\pi\omega_2)\cos(2\pi\omega_3)] \end{aligned} \tag{53}$$

$$\begin{aligned} V_5 = 4W_5[&\cos(3\pi\omega_1)\{\cos(\pi\omega_2)+\cos(\pi\omega_3)\}+\cos(3\pi\omega_2)\{\cos(\pi\omega_1)+\cos(\pi\omega_3)\} \\ &+ \cos(3\pi\omega_3)\{\cos(\pi\omega_1)+\cos(\pi\omega_2)\}] \end{aligned} \tag{54}$$

$$V_6 = 8W_6[\cos(2\pi\omega_1)\cos(2\pi\omega_1)\cos(2\pi\omega_1)] \tag{55}$$

$$\begin{aligned} V_7 = 8W_7[&\cos(3\pi\omega_1)\{\cos(2\pi\omega_2)\cos(\pi\omega_3)+\cos(\pi\omega_2)\cos(2\pi\omega_3)\} \\ &+ \cos(2\pi\omega_1)\{\cos(\pi\omega_2)\cos(3\pi\omega_3)+\cos(3\pi\omega_2)\cos(\pi\omega_3)\} \\ &+ \cos(\pi\omega_1)\{\cos(2\pi\omega_2)\cos(3\pi\omega_3)+\cos(3\pi\omega_2)\cos(2\pi\omega_3)\}] \end{aligned} \tag{56}$$

$$V_8 = 2W_8[\cos(4\pi\omega_1)+\cos(4\pi\omega_2)+\cos(4\pi\omega_3)] \tag{57}$$

The most convenient set of reciprocal lattice vectors for the FCC lattice is the set $\mathbf{a}_i^*$ that point along the three cube axes and have magnitude (1/a). In terms of these vectors the reciprocal vector, $\mathbf{A}_3^*$, to the (hkl) plane is

$$\mathbf{A}_3^* = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^* \tag{58}$$

A. The {111} Antiphase Boundary in the $L1_2$ Superlattice

The $L1_2$ structure is an ordering on the FCC lattice in which solute atoms occupy the corner positions in the FCC unit cell. It has the stoichiometric composition A_3B, and is assumed by a number of important intermetallic compounds, including γ' Ni_3Al and δ' Al_3Li. The solute distribution in the $L1_2$ structure is [Khachaturyan, 1978]

$$x^o(\mathbf{r}) = \bar{x} + \bar{x}\eta[e^{i\mathbf{k}_1\mathbf{r}}+e^{i\mathbf{k}_2\mathbf{r}}+e^{i\mathbf{k}_3\mathbf{r}}] \tag{59}$$

which has the form of equation (9) with

$$\mathbf{k}_j = (2\pi/a)\mathbf{e}_j \qquad (\mathbf{e}_j = [100],[010],[001]) \tag{60}$$

and

$$\gamma_i = \bar{x}\eta \tag{61}$$

For the (111) plane in the $L1_2$ structure the vector $\mathbf{A}_3^*$ is (1/a)[111], and

$$2\pi\xi\mathbf{A}_3^* = (2\pi/a)[\xi,\xi,\xi] \tag{62}$$

In this case $\Psi(\mathbf{k}_1) = \Psi(\mathbf{k}_2) = \Psi(\mathbf{k}_3)$, so we need evaluate only $\Psi(\mathbf{k}_1)$. The vector

$$2\pi\xi\mathbf{A}_3^* + \mathbf{k}_1 = (2\pi/a)[1+\xi,\xi,\xi] \tag{63}$$

has the form of equation (48) with $\omega_1 = (1+\xi)$, $\omega_2 = \omega_3 = \xi$. Using the definition (43) and equations (50)-(57), the series for the potential $\Delta V(\mathbf{k}_1,\xi)$ is, to the eighth neighbor interaction,

$$\begin{aligned}
\Delta V(\mathbf{k}_1,\xi) &= V(2\pi\mathbf{A}_3^*+\mathbf{k}_1) - V(\mathbf{k}_1) \\
&= -4W_1[\cos(2\pi\xi)-1] + 6W_2[\cos(2\pi\xi)-1] \\
&\quad - 8W_3[\cos(2\pi\xi)\cos^2(\pi\xi)-1] + 12W_4[\cos^2(2\pi\xi)-1] \\
&\quad - 8W_5[\cos(2\pi\xi)\cos(\pi\xi)-1] + 8W_6[\cos^3(2\pi\xi)-1] \\
&\quad - 16W_7[\cos(3\pi\xi)\cos(2\pi\xi)\cos(\pi\xi)-1] + 6W_8[\cos(4\pi\xi)-1] \\
&= \sin^2(\pi\xi)\{4W_1 - 12W_2 + 8W_3[2+\cos(2\pi\xi)] - 24W_4[1+\cos(2\pi\xi)] \\
&\qquad + 8W_5[3-2\cos(2\pi\xi)] - 4W_6[3-2\cos(2\pi\xi)+\cos(4\pi\xi)] \\
&\qquad + 16W_7[3+3\cos(2\pi\xi)+\cos(4\pi\xi)] - 24W_8[1+\cos(2\pi\xi)]\}
\end{aligned} \tag{64}$$

If equation (64) is substituted into equation (47) and integrated term-by-term the result is

$$\Psi(\mathbf{k}_1) = 2W_1-6W_2+8W_3-12W_4+12W_5-6W_6+24W_7-12W_8 \tag{65}$$

where we have used the identity

$$\begin{aligned}
\int_{-1/2}^{1/2} d\xi\{\cos(p\pi\xi)\sin^2(N_z\pi\xi)\} &= (1/2)\int_{-1/2}^{1/2} d\xi\{\cos(2p\pi\xi)[1-\cos(2N_z\pi\xi)\} \\
&= 0 \qquad (p < N_z)
\end{aligned} \tag{66}$$

which holds for all integers, p, less than N_z.

Note that equation (66) is only certain to hold when $r^\circ < D$. When the range of atomic interaction exceeds D then the series modifying W_i for large values of i may contain terms in $\cos(2p\pi\xi)$ with $p > N_z$. The integral does not vanish for these terms, and σ^A becomes dependent on the domain thickness. This result reflects the physical limitation that σ^A has its asymptotic value only when $r^\circ < D$ so that the boundaries of the domain do not interfere.

To complete the solution to equation (41) for the antiphase boundary energy we also need the area, s, per lattice site in the (111)

plane,

$$s = (\sqrt{3})a^2/4 \tag{67}$$

and the antiphase vector, **b**. There are, in fact, two possible values for **b**: $(a/2)[1\bar{1}0]$ and $(a/2)[11\bar{2}]$. However, both lead to the same value of the antiphase boundary tension, since the sum

$$\Sigma_j \sin^2(\mathbf{k}_j\mathbf{b}/2) = 2 \tag{68}$$

is the same in both cases.

The antiphase boundary energy for the (111) boundary in the $L1_2$ structure is evaluated by substituting equations (60), (61), (65), and (66)-(68) into equation (32). The result is

$$\sigma^A(111) = (16/a^2\sqrt{3})\bar{x}^2\eta^2[W_1-3W_2+4W_3-6W_4+6W_5-3W_6+12W_7-6W_8+\ldots] \tag{69}$$

When the $L1_2$ phase is perfectly ordered, $\bar{x}=1/4$ and $\eta=1$ and the antiphase boundary tension is

$$\sigma^A(111) = (1/a^2\sqrt{3})[W_1-3W_2+4W_3-6W_4+6W_5-3W_6+12W_7-6W_8+\ldots] \tag{70}$$

To test the validity of equation (70) we show that it reduces to the simple result obtained by Flinn [1960] when only nearest neighbor interactions are included, and then use it to compute the energy of a (111) antiphase boundary in Al_3Li. In the nearest neighbor model equation (80) becomes

$$\sigma^A(111) = (1/a^2\sqrt{3})W_1 \tag{71}$$

which reproduces the result obtained by Flinn [1960], who simply counted the number of wrong B-B bonds across a (111) boundary shifted by $(a/2)[1\bar{1}0]$. (To make the association, however, one must recognize that the the interaction energy used by Flinn [1960] is defined so that its value is $W_1/2$).

To estimate the energy of a (111) antiphase boundary in Al_3Li (δ') we use values for the interaction potentials $V(0)$ and $V(\mathbf{k}_1)$ that provide a fit to the metastable two-phase region between the ordered δ' phase and the disordered Al-Li solution [Khachaturyan, Lindsey and Morris, 1986]:

$$V(0) \cong 7\text{x}10^{-13} \text{ ergs} \tag{72}$$

$$V(\mathbf{k}_1) \cong -5.6\text{x}10^{-13} \text{ ergs} \tag{73}$$

These two values of $V(\mathbf{k})$ permit the computation of the first two interaction potentials from equation (49). The result is

$$W_1 \cong 7.9\text{x}10^{-14} \text{ ergs} \tag{74}$$

$$W_2 \cong -4.1\text{x}10^{-14} \text{ ergs} \tag{75}$$

Then, from equation (70),

$$\sigma^A(111) \cong 72 \text{ erg/cm}^2 \tag{76}$$

which is in reasonable agreement with the value obtained by Glazer and Morris [1986] from an analysis of available data on dislocation interactions.

B. The Tension of the (100) Boundary in the $L1_2$ and $L1_0$ Superlattices

The reciprocal vector, $\mathbf{A}_3^*$, for a (100) plane in the FCC lattice is

$$2\pi\mathbf{A}_3^* = (2\pi/a)[100] \tag{77}$$

The ordering vector $\mathbf{k}_1$ is perpendicular to the (100) plane, and hence perpendicular to the antiphase vector, $\mathbf{b}$, which lies in the plane. It follows from equation (32) that $\Psi(\mathbf{k}_1)$ does not influence $\sigma^A(100)$. Moreover, $\Psi(\mathbf{k}_2) = \Psi(\mathbf{k}_3)$ by symmetry. We therefore need only evaluate $\Psi(\mathbf{k}_3)$. Given the vector

$$2\pi\xi\mathbf{A}_3^* + \mathbf{k}_3 = (2\pi/a)[\xi 01] \tag{78}$$

the potential difference is

$$\Delta V(\mathbf{k}_3,\xi) = 4\sin^2(\pi\xi)\{-W_2+4W_3-4W_4-4W_6+8W_7-2W_8[1+\cos(2\pi\xi)]+\ldots\} \tag{79}$$

Substituting equation (79) into equation (47) and integrating term-by-term gives the result

$$\Psi(\mathbf{k}_3) = -2W_2+8W_3-8W_4-8W_6+16W_7-4W_8+\ldots \tag{80}$$

Given the antiphase vector across a (100) boundary in $L1_2$, $\mathbf{b} = (1/2)[011]$, and the area per lattice site, $s = a^2/2$, the tension of the

(100) antiphase boundary in the $L1_2$ structure is

$$\sigma^A(100) = (32/a^2)(\bar{x}\eta)^2[-W_2+4W_3-4W_4-4W_6+8W_7-2W_8+...] \quad (81)$$

In the completely ordered state, $\bar{x}=1/4$, $\eta=1$, and

$$\sigma^A(100) = (2/a^2)[-W_2+4W_3-4W_4-4W_6+8W_7-2W_8+...] \quad (82)$$

To compute the energy of a (100) antiphase boundary in the $L1_0$ (CuAuI) ordering on the FCC lattice we first require the solute distribution for $L1_0$, which is [Khachaturyan, 1978]

$$x^o(r) = \bar{x} + \bar{x}\eta e^{i\mathbf{k}_3 r} \quad (83)$$

It follows that there is only one ordering vector, $\mathbf{k}_3 = (2\pi/a)[001]$, with amplitude $\gamma_3 = \bar{x}\eta$. Since the $L1_0$ structure is also an ordering on FCC, the vector $\mathbf{A}_3^q$, the function $\Psi(\mathbf{k}_3)$, the area s, and the antiphase vector, **b**, have exactly the same values as they do for the (100) plane in the $L1_2$ superlattice. The antiphase boundary energy for the (100) plane in $L1_0$ is, hence,

$$\begin{aligned}\sigma^A(100) &= (1/s)|\gamma_3|^2\Psi(\mathbf{k}_3) \\ &= (16/a^2)(\bar{x}\eta)^2[-W_2+4W_3-4W_4-4W_6+8W_7-2W_8+...]\end{aligned} \quad (84)$$

For the completely ordered state,

$$\sigma^A(100) = (1/a^2)[-W_2+4W_3-4W_4-4W_6+8W_7-2W_8+...] \quad (85)$$

V. DISCUSSION

The solution derived above is, to our knowledge, the first analytic solution for the antiphase boundary energy that includes interactions beyond the second neighbor shell. It is convenient in the sense that it can incorporate the long-range interatomic interaction in either of two forms. Given the function V(k), which might be determined by diffuse x-ray scattering or calculated from the electron energy in momentum space, the tension of an arbitrary antiphase boundary can be found from equations (60) and (41). Given the real space interaction, W(r), the tension can be calculated from the series expansion in equation (62). In either case, the solution is relatively straightforward, as illustrated by the examples presented in the previous section.

However, the calculation does assume a sharp interface that is undisturbed by chemical relaxation or elastic distortion, and hence places an upper limit on the antiphase boundary tension. It seems obvious that chemical relaxations will occur in boundaries that reach equilibrium at moderate to high temperature; recent studies by Foiles [1986] and by Sanchez, et al. [1986] suggest that this is the case in Ni_3Al. Chemical redistributions near an equilibrium boundary should be less important at low temperature, and, for kinetic reasons, should not contribute significantly to the tension of an antiphase boundary that is formed at moderate temperature by the passage of a partial dislocation. The latter case is of significant practical interest since it governs the strength of intermetallic compounds and the hardening achieved by ordered precipitates at moderate temperature.

The calculation also assumes a pairwise interatomic interaction, or, more specifically, a pairwise reconfiguration potential for the solute species. The issue of the interatomic potential has recently been investigated by Stocks, et al. [1986], for various intermetallic compounds. Their results suggest that a pairwise interaction is reasonable for some systems, but may lead to significant errors in treating the ordering behavior of others [Stocks, 1986]. Since the antiphase boundary is a perturbation on a phase that is already ordered, it is not clear how important many-body interactions may be in the present case.

The theory was applied to obtain one numerical result, for a (111) antiphase boundary in δ' Al_3Li. The result obtained, ~ 72 ergs/cm^2, should be compared to the value 57±15ergs/cm^2 found by Glazer and Morris [1986] from an analysis of dislocation interactions with δ' precipitates in Al-Li alloys. Given that the calculation ignores interactions beyond the second neighbors, that the values of the interaction parameters W_1 and W_2 are only approximately known, and that there are also approximations in the dislocation-interaction approach [Glazer, 1986; Glazer and Morris, 1986] the agreement seems reasonable.

However, the calculated value for the (111) boundary in δ' Al_3Li differs significantly from theoretical values reported elsewhere [Furukawa, et al., 1985; Jensrud, 1986]. The source of the discrepancy is relatively easy to identify. The method of calculation used by these authors ultimately traces back to the nearest-neighbor model used by Flinn [1960]. As noted by Marcinkowski [1963], the Flinn equation can be re-expressed in terms of the ordering temperature, T_0, which is, in a mean field model with nearest neighbor interactions (the Bragg-Williams model),

$$kT_0 = 0.82W_1 \tag{86}$$

Using equation (71) the (111) antiphase boundary energy can be written

$$\sigma^A(111) = kT_0/(\sqrt{3})0.82a^2 \tag{87}$$

This result was, however, misstated in later work [Copley and Kear, 1967] from which the more recent presentations are drawn. Part of the confusion probably arose from the fact that the interaction potential used by Marcinkowski [1963] is twice that defined by Flinn [1960]. The consequence was to introduce fairly large errors into the nearest-neighbor result. For example, the equation written by Jensrud [1986] is in error by a factor of 4; correcting the error reduces the value reported, 160 ergs/cm^2, to 40 ergs/cm^2, which is in much more reasonable agreement with the present results.

Unfortunately, it is not possible to relate the antiphase boundary energy to the ordering temperature when long-range interactions are taken into account. The ordering temperature for an $L1_2$ phase in the mean field approximation is [Khachaturyan, 1978]

$$kT_0 = 0.205[-4W_1+6W_2-8W_3+12W_4-8W_5+8W_6-16W_7+6W_8+...] \tag{88}$$

which is not a simple multiple of $\sigma^A(111)$ as given in equation (83).

Finally, we should mention the implications of the antiphase boundary energy for the stability of the ordered phase. Two relevant aspects of structural stability are governed by the antiphase boundary energy. The first is the stability with respect to the spontaneous formation of antiphase boundaries. If σ^A is negative for any plane then the ordered phase is unstable with respect to the formation of antiphase boundaries parallel to that plane. There appear to be ordered structures for which this is the case, and their interesting behavior is being explored.

The second relevant instability arises when the antiphase boundary tension is more than twice that of an interface between the ordered structure and the disordered parent lattice. In this case the antiphase boundary is unstable with respect to the formation of a film of disordered phase. This situation apparently applies in the case of δ' Al-Li, for which the precipitate-matrix boundary energy is of the order 20 ergs/cm^2 [Bauman and Williams, 1985] and also applies to γ' Ni_3Al, at least at elevated temperature. In the latter case disordered films have been observed along antiphase boundaries [Cahn, 1986].

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