Ising Model for Phase Separation in Alloys with Anisotropic Elastic Interaction. II. A Computer Experiment

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Abstract

When a metallic alloy is quenched into a miscibility gap, a mixture of two phases develops, whose domain structure then coarsens because of the interfacial energy between the two phases. This spatial arrangement of the domains and the rate at which they evolve may be strongly influenced by elastic interactions. In a recent paper the authors described a method for simulating the effect of anisotropic elastic interactions in a two-dimensional Ising model of a cubic alloy, using Kawasaki dynamics with the elastic interactions represented by a long-range two-body interaction potential. Here we present the results of such simulations at various temperatures, alloy compositions and misfits (by "misfit" we mean the difference in size between the two kinds of atom), exhibiting snapshots both of the microscopic configurations (corresponding to experimental measurements using transmission electron microscopy) and of their squared Fourier transforms (corresponding to measurements using small-angle X-ray or neutron scattering). The anisotropy of the two-phase structure increased with time, with misfit, and with composition, but decreased with increasing temperature. The rate of coarsening of the domains was found, surprisingly, to be roughly independent of the misfit at a given value of T/T_c.

1 Introduction

The coarsening of precipitates is an important phenomenon in alloys, since the size, shape and arrangement of the precipitates is a decisive factor for their mechanical properties. In two-phase mixtures, coarsening usually has the effect of reducing the total amount of interface between the phases. The process is quite well understood in liquid and in solid mixtures where the interface energy is the only driving force [2, 3, 4]. In alloys where the two pure phases have different lattice spacings, the problem is more complex because elastic misfit interactions (usually anisotropic) come into play. Hence, the precipitates may not be spherical, but rather cuboidal or plate-like, and may form ordered arrays [3, 5, 6, 7, 8, 9]. In some cases, a change in the rate of coarsening has also been reported [8, 10, 11].

Various theoretical approaches to this problem have been used: one of them is to calculate the elastic energy of one or more inclusions using continuum elasticity [12, 13, 14, 15, 16, 17, 18]; another is to use a Ginzburg-Landau type energy functional [19, 20, 21, 22, 23, 24, 25]; yet another uses microscopic models with isotropic elasticity [26, 27]. In order to be able to simulate coarsening on an atomic level in anisotropic alloys with large elastic misfit, we have introduced recently [1] (in a paper which will be referred to as I) a version of the Ising model which includes anisotropic elastic interactions. In this model, A and B atoms of different sizes are distributed near the sites of a square lattice. The atoms interact through a nearest-neighbour "inelastic" potential (as in the usual Ising model) which depends onlly on the identities (A or B) of the two atoms and not on their displacements from their lattice sites, and through an additional "elastic" potential which does depend on these displacements. The "elastic" potential is equivalent to a set of springs which connect nearest-neigbour and next-nearest neighbour pairs and are joined to them at the surfaces of the atoms (regarded as spheres of radius R_A or R_B). The displacements of the atoms are then chosen to minimize the elastic energy, and the resulting minimum energy turns out to be equivalent to a long-range anisotropic two-body interaction. The mean-field treatment in I predicts that as the misfit is increased from zero the domains will cease to look like randomly arranged droplets but will tend instead to form periodic stripes. In particular, in alloys with an elastic anisotropy like that of copper or nickel, the domains are predicted to be parallel to the (10) and (01) directions of the lattice.

In the present work, we show results of computer simulations for this modified Ising model at several temperatures and alloy compositions and at three different values of a parameter λ measuring the amount of misfit. Our main result is that the domains are more anisotropic, the larger the lattice misfit. Moreover, the anisotropy is larger for larger volume fractions of the precipitate and at lower temperatures. Surprisingly, the size of the domains remains proportional to the cube root of the time and, at fixed T/T_c, the proportionality coefficient is roughly independent of the amount of misfit.

2 The model

The Hamiltonian of our modified Ising model is given by eq.(19) in I as

$$E = W_0 + \frac{1}{2} \sum_{\mathbf{p}} \sum \mathbf{p}' \, \psi(\mathbf{p} - \mathbf{p}') \, \gamma(\mathbf{p}) \, \gamma(\mathbf{p}') \tag{1}$$

where $\gamma(\mathbf{p})$ is 1 if the occupant of site $\mathbf{p}$ is an A atom and -1 if it is a B atom, and ψ is the sum of a nearest-neighbour interaction term and an elastic interaction contribution ϕ due to the difference in sizes between the two kinds of atom (eqs 20 and 24 in I):

$$\psi(\mathbf{p}) = \begin{cases} (R_A - R_B)^2\phi(\mathbf{p}) - J & \text{if } \mathbf{p} \text{ connects nearest neighbours} \\ (R_A - R_B)^2\phi(\mathbf{p}) & \text{otherwise} \end{cases} \tag{2}$$

Here J is half the excess nearest-neighbour interaction energy of an A-B pair (as in the usual Ising model with nearest neighbour interaction) and R_A, R_B are the radii of the A and B atoms. The long-range elastic interaction potential $\phi(\mathbf{p})$ depends on the stiffnesses of the springs, which can be expressed in terms of the elastic constants c_{11}, c_{12} and c_{44} (eqs.(12), (21), (13) in I). The relative values of these constants, and of the elastic anisotropy ratio $A = 2\,c_{44}/(c_{11} - c_{12})$, are shown in Table 1 for a few common metals.

In our simulations, we chose to use the elastic constants for copper (first column in Table 1), a highly anisotropic material whose relative elastic constants are quite close to those of other important metals, such as nickel or iron. The size of the elastic misfit energy relative to the "inelastic" energy can be measured by a dimensionless parameter λ (introduced in I):

$$\lambda = (R_A - R_B)^2\; B/J \tag{3}$$

where B is the two-dimensional bulk modulus defined by $B = (c_{11} + c_{12})/2$.

To relate λ to quantities that can be measured in experiments, we define the lattice misfit δ as

$$\delta = (a_A - a_B)/a \tag{4}$$

where a_A and a_B are the lattice spacings of pure A and pure B phases and a is the lattice spacing of the alloy. The interfacial tension σ at zero temperature and zero misfit is the energy of an A-B bond divided by the amount of surface per bond

$$\sigma = 2J/a \tag{5}$$

The constant λ may then be written as

$$\lambda = \lambda_0\; \delta^2\, a\, B/\sigma \tag{6}$$

where

$$\lambda_0 = 2[(R_A - R_B)/(a_A - a_B)]^2 \quad . \tag{7}$$

It can be shown, using eqns (3) and (A9) of I, that λ_0 is equal to $\frac{1}{2}[(L_+ + L_\times)/(L_+ + \sqrt{2}L_\times)]^2$ where L_+ and $L_\times$ are the longitudinal stiffnesses of the springs along and diagonal to the lattice bonds. In terms of elastic constants their values are $L_+ = c_{11} - \frac{1}{2}(c_{12} + c_{44})$ and $L_\times = \frac{1}{2}(c_{12} + c_{44})$. For the elastic data used in our simulations, $\lambda_0 = 0.8145$. Since λ_0 depends on the elastic constants only, λ is proportional to the square of the misfit δ.

In the simulations, we used three values of λ: 0, 2.18 and 10.9. Assuming a typical lattice spacing $a \approx 0.4$nm, a bulk modulus $B \approx 2 \times 10^{11}$N/m^2 [?] and an interface tension $\sigma \approx 10^{-2}$N/m [?] for a real three-dimensional alloy these choices correspond, according to eqn (6), to lattice misfits of about 2% and 5% respectively. Such values are rather large, since domains with a linear dimension of 50 lattice spacings in one case, 20 in the other, would accumulate a total strain of one lattice spacing, so that misfit dislocations (which are not considered here) might be expected to appear by the time the domains reach such sizes. Provided the domain sizes remain less than about 10 lattice spacings, however, such dislocations should not occur and the assumption of a regular underlying lattice, upon which our theoretical treatment depends, should remain valid. Since on our small model lattice (64x64) the need to avoid finite size effects limits us anyway to configurations where the domains are smaller than about 10 lattice spacings, the choice of these rather large values of λ seemed appropriate so as to enhance the effects of elastic interaction.

3 Results of the simulations

Our simulations were performed on a SUN workstation using the algorithm for Kawasaki dynamics outlined in I. Runs at various temperatures and alloy compositions were started with (independent) random configurations and stopped after a given time t, measured in Monte-Carlo steps (MCS), i.e. the number of attempted exchanges per lattice site.

3.1 Critical temperature

For $\lambda = 0$, the critical temperature is the Onsager value $T^\star$, given by

$$k_B T^\star / J = 2/\ln(\sqrt{2}+1) \approx 2.27 \tag{8}$$

In I it was shown that the mean-field critical temperature (which in the case $\lambda = 0$ is $4\,J/k_B$) increases with λ by a factor of about $1 + 0.06\lambda$. The same critical temperature would be obtained by replacing the Ising model with long-range interaction by another with nearest neighbour interaction only and with J replaced by $J(1+0.06\lambda)$. Assuming that the true critical temperature T_c depends on λ in the same way as the mean-field critical temperature $T^\star$, one may thus expect T_c to behave approximately as

$$T_c \approx T_c^E(\lambda) \stackrel{\text{def}}{=} (1+0.06\lambda)\,T^\star \tag{9}$$

In order to verify this, we determined the total energy in a series of Monte-Carlo runs at various temperatures around T_c^E at times 10^2, 10^3 and 10^4 MCS. The result for $\lambda = 2.18$ is shown in Fig 1. It is clearly visible that for $T > 1.1\,T^\star$ the total energy does not decrease after time 10^3 MCS, indicating the presence of an equilibrium structure; on the other hand for $T \leq 1.1\,T^\star$ it continues to decrease until at least 10^4 MCS, probably because spinodal deomposition is in progress. Although this is not a very precise way to determine critical temperatures [28], this simulation nevertheless supports the conjecture (9) for $\lambda = 2.18$ and $\lambda = 10.9$, within a precision of 10%.

3.2 Morphology

The conditions under which simulations for studying the domain structure were performed are summarized in Table 2. The time evolution was investigated for three values of the elastic misfit parameter, namely $\lambda = 0$, 02.18 and 10.9, and various values for the concentration c. Some of the sets of runs were conducted at a fixed temperature T, but others were done at a fixed value of $T/T_c^E(\lambda)$ in order to correct for the change of the equilibrium phase diagram with λ at fixed T.

Snapshots illustrating the morphological evolution at a fixed value of T are shown in Figs.2-5, where (a) gives the actual configuration (as it would be observed in, e.g., electron microscopy), (b) gives its absolute squared Fourier transform (corresponding to an observation of small-angle scattering using a single crystalline sample) and (c) gives the radial average of (b) (corresponding to small-angle scattering from a polycrystal).

Figure 2a shows three series of snapshots illustrating the time evolution of the configuration at concentration (of, say, A atoms) $c = 0.5$ and temperature $T = 0.5T^\star$. For $\lambda = 0$ (left column) the structure stays isotropic as it coarsens, but for $\lambda > 0$ there is a definite preference for stripes along rows or columns of the lattice, this preference being the most pronounced for the largest misfit (right column of the diagram). This preference is not unexpected, since the rows and columns correspond to the elastically soft directions in this system. In addition, the stripes are arranged roughly periodically, so that not only the orientational ordering but also the positional ordering increases with increasing λ. Moreover, the increase of λ also slows down the coarsening (this is best visible in the bottom row of Fig.2a). One must, however, be very careful in interpreting this last result, since the phase diagram also changes with λ. In fact, in Fig. 2a the relative temperature T/T_c^E is only 0.3 for $\lambda = 10.9$, while it is 0.5 for $\lambda = 0$. This change in T/T_c^E may account for at least part of the slowing down as λ is increased..

Fig. 3a shows a similar series of snapshots, done this time at a fixed *relative* temperature $T/T_c^E = 0.8$, so as to allow for the change in T_c^E with λ required by eq (9). Again the same morphological effects as in Fig.2 are visible. The interfaces are somewhat noisier due to the increased temperature. But note that in Fig.3a the size of the domains at a given time is roughly the same for all three values of λ. Hence, most of the change in the rate of coarsening visible in Fig.2 was due to the change of the equilibrium phase diagram.

A further effect visible in Fig. 3a is the symmetry breaking for $\lambda = 10.9$ at the latest time, all the stripes being vertical.

Figs. 2b and 3b show the squared moduli of the Fourier transforms of the configurations in Fig.2a and 3a, defined as

$$I(\mathbf{k}) = |\sum_{\mathbf{p}} \gamma(\mathbf{p})\, e^{i\mathbf{k}\cdot\mathbf{p}}|^2 \tag{10}$$

These pictures would correspond to measurements of the small-angle scattering (SAS) using single crystals. For $\lambda = 0$, a ring is clearly visible, which shrinks with time. In this case the Fourier transforms are isotropic. This isotropy of the SAS pattern is consistent with the empirical self-similarity law (dynamical scaling) observed in other studies ([4]), according to which $I(\mathbf{k}, t)$ is proportional to a power of t times a universal function of $|\mathbf{k}|t^{1/3}$. The situation is quite different for $\lambda = 2.18$ (centre column). Here, even at the earliest time shown, the SAS is not isotropic; it shows instead a flower-like pattern, with the leaves along rows and columns of the lattice. Some coarsening is also visible as time increases, in the form of a shrinkage of the pattern. The anisotropy is even more pronounced at $\lambda = 10.9$ and here there is clearly no scaling when the domain structure coarsens; the streaks become markedly sharper with time, indicating an increasing anisotropy. Moreover, in Fig 3b at the latest time most of the intensity is concentrated in a horizontal stripe; this is a manifestation of the symmetry breaking already noted in Fig.3a. The shape of the SAS pictures at early times in Fig.2b and 3b mimics the shape of the **k**-space potential $\psi(\mathbf{k})$, as depicted in Fig.2 in I. Also these figures agree well with the patterns predicted by the mean-field theory presented in I (Fig.5 in I).

Figs.2c and 3c show radial averages of these SAS patterns. Such averages would correspond to measurements using polycrystals. At $\lambda = 0$, a peak is visible, shifting with time towards smaller **k**. This is the usual behaviour of the structure function in phase separation with negligible elastic misfit interactions [4, 2]. When $\lambda > 0$, on the other hand, the peak becomes considerably sharper with time without any corresponding shift in the maximum, particularly in the right-hand column of Fig. 3c. This strongly non-scaling behaviour shows that the elastic interactions cause the positional order of the domains to increase with time.

In addition to the computation illustrated in Fig.3, we did similar ones at two other concentrations (of, say, A atoms): $c = 0.4$ and $c = 0.25$. For $c = 0.4$ most of the conclusions are the same as for $c = 0.5$, but for $c = 0.25$ some new effects occur. These are illustrated in Fig.4. Fig.4a shows snapshots of the configurations, in which the minority phase now coagulates into lumps or "precipitates". For $\lambda = 0$ the precipitates are more or less round (left-hand column), but for $\lambda = 10.9$ they are definitely needle-shaped. In the intermediate case $\lambda = 2.18$, they are not needle-shaped but somewhat elongated along lines or columns of the lattice. What is most striking, however, is that when $\lambda > 0$ the precipitates are arranged in an almost periodic fashion. The Fourier-transformed patterns (Fig.4b) are rather similar to the ones for $c = 0.5$ (Fig.3b) although noisier because of the smaller concentration c. In the radially averaged patterns (Fig.4c), however, a new effect appears: in the right column an oscillation superimposed on the structure function is clearly visible. Qualitatively this result may be understood as follows: As a first approximation, the structure function may be considered as the product of the form factor due to the individual precipitates and a factor describing the correlation in position of different precipitates [29]. Hence, the broad component of the structure visible in Fig.4c is due to the form factor of the (relatively small) precipitates. The periodic arrangement of the precipitates (the separation between precipitates being several times larger than their thickness) then modulates this broad component at a smaller wavelength which corresponds to the separation of the precipitates. Indeed, several orders of such an oscillation can be seen in the right column of Fig.4c. The reason why this effect is not apparent in Fig.3c ($c = 0.5$) is that in this case the distance between precipitates turns out to be just twice their thickness, so that the second order of the oscillation is cancelled. The remaining pattern consists mainly a sharp first order peak (see Fig.3c bottom right) with only a trace of higher orders.

3.3 Kinetics

The kinetics of domain growth can be analyzed by plotting the domain size R (defined here as the first zero of the two-point correlation function, i.e. the Fourier transform of the radially averaged I($\mathbf{k}$)), versus time (Fig.5). In the nearest-neighbour Ising model the resulting graph can be represented [30, 2] by

$$R = R_0 + a\,(t/t_0)^{1/3} \tag{11}$$

where a is the lattice spacing and R_0 and t_0 are constants[1]. To compare the kinetics for different values of λ, we have plotted R/a versus $t^{1/3}$ in Fig.5. The data were fitted using eq.(11) and the constants R_0 and t_0 obtained in the fit are listed in Table 3. Four conclusions can be drawn from Fig.5 and Table 3.

1. Eq. (11) fits the data for $\lambda > 0$ and for $\lambda = 0$ equally well. This shows that in this mode the elastic misfit interactions with anisotropic but homogeneous elastic constants do not qualitatively change the growth law. In particular, there is no slowing down at a critical size (as found experimentally in some alloys [10, 8]), despite the considerable changes in the morphology due to the misfit interactions.

2. For a given temperature the rate of growth depends very little on the composition. This is known for the Ising model without elastic misfit [32], but appears to remain true even when it is present.

3. The intercept of the straight lines in Fig.5, R_0/a, is almost the same in all cases, (in fact R_0/a lies between 2 and 3 for all the data in Fig.5).

4. While the slope t_0^{-1} increases significantly with λ (by a factor of more than 100) at a given *absolute* temperature ($T = 0.5T^\star$) in Fig.5 and Table 1, the variation with λ at a given *relative* temperature T/T_c^E is much less.

To sum up: with or without elastic interactions, the growth of R with time is given by eqn (11), and the parameters a and t_0 are approximately independent of the concentration c and the misfit parameter λ at constant relative temperature T/T_c^E.

This last observation is rather surprising, since it would indicate that the elastic interaction influences only the evolution of shape and position of the domains and not that of the total amount of interface separating them. To test this conclusion further, we investigated the fraction f_{AB} of A-B nearest neighbour pairs,

$$f_{AB} = \frac{1}{2} - \frac{1}{4N} \sum_{\{\mathbf{p},\mathbf{p}'\}} \gamma(\mathbf{p})\,\gamma(\mathbf{p}') \tag{12}$$

which is a crude estimate of the total amount of interface. Here N is the number of lattice sites and the sum extends over all nearest-neighbour pairs. Fig.6 shows f_{AB} plotted as a function of a/R for all data in Fig.5. It turns out that regardless of composition and temperature an approximate relation

$$f_{AB} \approx \frac{3}{2}\,\frac{a}{R} \tag{13}$$

holds in the case of $\lambda = 0$ and $\lambda = 2.18$. For the very large misfit $\lambda = 10.9$, the data are more scattered, but the same relation still gives a rough representation. Hence, we find that the total amount of interface is, indeed, roughly proportional to $1/R$ in all cases regardless

[1]This does not quite correspond to the growth law derived by Lifshitz, Slyozov and Wagner (LSW theory [31]) where R^3 should grow linearly with time. Only in the limit of very large R are the two growth laws equivalent. A possible reason for this transient deviation of the dynamic Ising model from LSW theory may be a curvature dependence of the interfacial tension [32].

of the elastic misfit. Consequently, the conclusion drawn in the preceding paragraph about the growth of R applies in the same way to the inverse of the total amount interface between domains.

3.4 Anisotropy

To study the time dependence of the anisotropy of the domain patterns, we first use the structure function $I(\mathbf{k}) = I(k, \theta)$, where the zero of the polar angle θ is taken along a (10)-direction of the lattice, to define:

$$J_n = \int_{(2n-1)\pi/8}^{(2n+1)\pi/8} d\theta \int_0^{\pi/a} dk\, I(k, \theta) \qquad (n = 0, \ldots, 7) \tag{14}$$

As a measure of the anisotropy we use a parameter α which characterizes the deviation from radial symmetry:

$$\alpha = \sum_{p=0}^{3} (J_{2p} - J_{2p+1}) \; / \; \sum_{n=0}^{7} J_n \tag{15}$$

In Fig.7, we have plotted α as a function of domain size R/a for (a) $\lambda = 0$, (b) $\lambda = 2.18$ and (c) $\lambda = 10.9$. Clearly α has to be close to 0 when there are no elastic interactions ($\lambda = 0$), and this is evident – apart from fluctuations – in Fig.7a. Several results emerge from a study of Figs.7b and 7c:

1. In all cases the anisotropy increases (continuously) with R, but the system is strongly anisotropic from the very beginning. There is no critical value of R at which previously isotropic precipitates become anisotropic, contrary to the theories proposed in [5] and [15].

2. At fixed composition and temperature, the anisotropy is larger for larger misfits.

3. For given temperature and misfit the anisotropy decreases as c decreases from 0.5 to 0.2.

4. For given composition and lattice misfit the anisotropy decreases with temperature.

Hence, the largest anisotropy is to be expected from a symmetric ($c = 0.5$) alloy with large misfit at low temperatures. In terms of mean-field theory, this temperature dependence can be understood by saying that the entropy term in the free energy tends to produce isotropy, while the internal energy term tends to produce anisotropy — as the temperature is lowered, the anisotroppic energy term becomes relatively more important.

Since symmetry breaking was observed in a few cases (such as in Fig. 3a, bottom right) we also define a parameter η which characterizes the breaking of cubic symmetry:

$$\eta = \sum_{p=0}^{1} (J_{4p} - J_{4p+2}) \; / \; \sum_{p=0}^{3} J_{2p} \tag{16}$$

In Fig.8 η and $1 - \eta$ are plotted together as a function of domain size R. It is apparent from Fig.8a that there is no symmetry breaking when $\lambda = 0$. For large R, the asymmetry

η increases up to values close to 0.5 when $\lambda = 2.18$, but this increase may be due to fluctuations. At $\lambda = 10.9$, however, there is a clear bifurcation near $R = 10$, where the pattern switches to stripes in either a horizontal or vertical direction. In fact, looking at the right-hand column of Fig.3a, one can see that even before this symmetry breaking of the parameter η there are some regions where the stripes are mostly horizontal and others where they are mostly vertical. These regions appear to become larger with time, and eventually when their size is near enough to the system size there is a bifurcation towards a single region with either horizontal or vertical stripes onlly. Thus one may expect the actual R-value where bifurcation occurs to depend on the system size. This last hypothesis could be tested by doing computer experiments on lattices of different sizes.

Finally, we wanted to check whether the anisotropy α behaves in a universal way when plotted versus a typical length scale characterizing the sizes of the domains [15, 9]. A possible length scale for this purpose is

$$L = c_{44}\, \delta^2\, R \,/\, \sigma, \tag{17}$$

a combination of elastic constant, interface tension and domain size, which by (6) is proportional to $\lambda R/a$ (since B and c_{44} are fixed in our simulations). Curves of α against $\lambda R/a$ did not, however, superimpose for different values of the misfit parameter λ. We then tried replacing $\lambda R/a$ by

$$\Lambda = \lambda(R - R_0)/a \tag{18}$$

where R_0 is a constant to be chosen. Fig.9 shows α plotted against Λ for $\lambda = 2.18$ and 10.9 and for several compositions at the same relative temperature of $T/T_c^E = 0.8$. There is a reasonable superposition of the data when $R_0 = 2.5$. Note that this is exactly the value for the the domain size extrapolated to time 0 using eq.(11) (i.e., the constant in Table 3). The data illustrated in Fig.9 are all for the same (relative) temperature, because for different temperatures the curves did not superimpose. Fig.9 also shows a clear dependence of the curve on composition c. Therefore, even though α varies with the length scale Λin a way that is "universal" with respect to the amount of misfit, the curve so obtained still depends on both composition and temperature.

4 Conclusion

Our results show that, for spinodal decomposition in the two-dimensional Ising model, the introduction of elastic misfit strains with negative cubic anisotropy strongly changes the shapes of the domains. They tend to be elongated or even stripe-like along the (10) or (01)-directions. Their positions also tend to be more regularly distributed than in the case without misfit. This is particularly visible at small alloy compositions (like $c = 0.2$), where the precipitates align along (10) and (01) directions. A quantitative evaluation shows that, within this model system, the domains are anisotropic from the very beginning of decomposition and become more so with time. There is no bifurcation from spherical to anisotropic particles as proposed in some theoretical treatments [5, 15, 8]. Moreover, the anisotropy increases when the concentration increases (towards $c = 0.5$) or the temperature decreases. Finally, regions with parallel stripes develop and grow larger with time, so that eventually only one variant (horizontal or vertical stripes) may be present on the (finite) lattice, thus effectively breaking the cubic symmetry.

All these morphological effects are rather similar to the ones observed experimentally in some alloy systems, such as the nickel-based superalloys [6, 9, 8]. Our results also indicate that the rate of growth of the domains in the Ising model does NOT increase with increasing lattice misfit, if one keeps the equilibrium phase diagram fixed. In particular, the growth law ($R \propto t^{1/3}$, eq.11) of the domain size R is always observed, regardless of the misfit. This again is not unlike the case of nickel-based superalloys, where no deviation from the $t^{1/3}$ law was found experimentally [9].

Thus, if only elastic anisotropy (but no inhomogeneity, i.e. no dependence of the elastic coupling constants on the local alloy concentration) is considered, there is no change in the overall growth law of the domain thickness, even though strong changes in the morphology occur due to elastic misfit strains. The strong slowing-down of coarsening found in some alloys with misfitting precipitates [10, 8] appears to arise mostly from inhomogeneity (different values for the elastic constants in the two phases) [33] rather than from the anisotropy considered here.

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Figure Captions

Figure 1: Dependence of the total energy on temperature for configurations obtained after 10^2 (disks), 10^3 (squares) and 10^4 (triangles) MCS (Monte-Carlo steps) starting from a random distribution of A and B atoms. The composition was $c = 0.5$ and the misfit parameter was $\lambda = 2.18$. The arrow shows the temperature T_c^E as defined in (9).

Figure 2: **(a)** Snapshots of configurations for $c = 0.5$ and $T/T^\star = 0.5$ (conditions as indicated in Table 2: columns from left to right are, respectively, for $\lambda = 0$, $\lambda = 2.18$ and $\lambda = 10.9$). Rows from top to bottom: $t = 250$ MCS, $t = 4000$ MCS, $t = 64000$ MCS. These pictures correspond to "measurements" using transmission electron microscopy.
(b) Squared Fourier transforms of pictures in (a). These correspond to "measurements" using single crystal small-angle scattering.
(c) Radial average of the pictures in (b). These correspond to "measurements" using polycrystal small-angle scattering.

Figure 3: As Figure 2, but with $c = 0.5$ and $T/T_c^E = 0.8$ (see Table 2). and with rows from top to bottom: $t = 250$ MCS, $t = 2000$ MCS, $t = 16000$ MCS.

Figure 4: As Figure 2, but with $c = 0.2$ and $T/T_c^E = 0.8$ (see Table 2). and with rows from top to bottom: $t = 125$ MCS, $t = 1000$ MCS, $t = 8000$ MCS.

Figure 5: Domain size R (in units of lattice spacing a) as a function of time t. Symbols are defined in Table 3. The full lines are fitted to the data points using eq.(11) and the parameters given in Table 3.

Figure 6: Fraction f_{AB} (eq.12) of nearest-neighbour A-B bonds as a function of domain size R. Symbols are defined in Table 3. The full lines all correspond to eq.(13).

Figure 7: Anisotropy α as a function of domain size R. The symbols are defined in Table 3. Full lines are guide to the eye.

Figure 8: Asymmetry η as a function of domain size R. The symbols are defined in Table 3.

Figure 9: Anisotropy α as a function of $\lambda(R - R_0)/a$, where $R_0/a = 2.5$. Symbols are defined in Table 3.

Table 1:

Table 1: Relative elastic constants for some common metals. The two-dimensional bulk modulus is $B = (c_{11} + c_{12})/2$ and the anisotropy ratio is $A = 2\,c_{44}/(c_{11} - c_{12})$.

	Cu	Ni	Fe	Al	W
c_{11}/B	1.16	1.22	1.25	1.27	1.43
c_{12}/B	0.84	0.78	0.75	0.73	0.57
c_{44}/B	0.52	0.58	0.61	0.33	0.33
A	3.21	2.63	2.42	1.22	0.76

Table 2:

Table 2: Conditions at which the Monte-Carlo experiments were performed. For each condition, 8 runs were started from independent random distributions of A and B atoms and stopped after $1000 * 2^i$ MCS (where $i = -3, ..., 4$). The first column indicates the figure comprising the relevant snapshots.

figure	composition	temperature		misfit (eq.6)
	c	$T/T^\star$	T/T_c^E	λ
	0.5	0.5	0.5	0
2	0.5	0.5	0.44	2.18
	0.5	0.5	0.3	10.9
	0.5	0.8	0.8	0
3	0.5	0.9	0.8	2.18
	0.5	1.3	0.8	10.9
	0.2	0.8	0.8	0
4	0.2	0.9	0.8	2.18
	0.2	1.3	0.8	10.9

Table 3:

Table 3: Constants R_0 and t_0 obtained by fitting the average domain size R shown in Fig.6 to the formula eq.(11). Definition of the symbols for figures 5 to 9.

condition				equation (11)		symbols in Figs. 5-9	
λ	T/$T^{\star}$	T/T_c^E	c	R_0/a	$t_0(MCS)$	colour	shape
0	0.5	0.5	0.5	2.26	2.4×10^2	grey	circle
2.18	0.5	0.4	0.5	2.76	2.6×10^4	white	circle
10.9	0.5	0.3	0.5	2.24	7.2×10^4	black	circle
0	0.8	0.8	0.5	2.26	4.6×10^1	grey	square
2.18	0.9	0.8	0.5	2.44	1.1×10^2	white	square
10.9	1.3	0.8	0.5	2.64	4.8×10^2	black	square
0	0.8	0.8	0.4	2.23	5.5×10^1	grey	diamond
2.18	0.9	0.8	0.4	2.93	2.9×10^2	white	diamond
10.9	1.3	0.8	0.4	2.21	1.3×10^2	black	diamond
0	0.8	0.8	0.2	2.12	4.1×10^1	grey	triangle
2.18	0.9	0.8	0.2	2.38	1.0×10^2	white	triangle
10.9	1.3	0.8	0.2	3.04	2.6×10^2	black	triangle