A. Kumar et al.: Critical sizes for coherent to semicoherent transition in precipitates

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1. Introduction

On growth beyond a critical size, a coherent precipitate can become semicoherent through the formation of interfacial misfit dislocations. This investigation pertains to the finite element simulation of the state of stress of a coherent precipitate, its growth and the change in state of stress on the formation of an interfacial misfit dislocation loop. Critical radii are determined from the simulations based on: (i) global energy minimum \( r^* \) and (ii) local force balance along the radial direction \( r_2 \). The concept of local force balance as existing in literature is extended to the circumferential direction, to calculate a new critical size \( r_2 \). Local force balance gives radii at which the interface is the stable position for the dislocation loop. Off-interface stability of the dislocation loops is also investigated. The Cu–γFe system is used as an example to illustrate the new methodology developed and validate the results of the simulation. The power of the methodology is shown by considering a configuration (precipitation in a thin disc), where standard theoretical formulations are inadequate.

Keywords: Coherent precipitate; Interfacial misfit dislocation; Critical size; Finite element method

Finite element method (FEM) has proved to be a useful tool in the study of various aspects regarding dislocations and precipitation process. Stigh [5] used FEM for the study of threading dislocations. Sasaki et al. [6] have obtained the stress fields of an edge dislocation, using a finite element technique involving the removal of a plane of atoms. Techniques of simulation of dislocations at the mesoscopic scale have also been developed [7, 8]. FEM has successfully been used for the simulation and study of the precipitation process in various systems. The strain energy increase associated with precipitation [9] and the morphology of the precipitates [10] have been analyzed using FEM. The technique has also been proved useful in the determination of stresses associated with phase transformations [11] and in the study of long-range internal stresses in superalloys [12]. Precipitation in epitaxial films has also been studied by means of FEM [13]. Various aspects of inclusions, including the stress state around them, have also been studied using FEM [14, 15] and extended FEM (X-FEM) [16, 17]. From a mechanics perspective an inclusion can be treated equivalent to a precipitate. FEM has also been used for the study of other coherent nanostructures such as epitaxial films [18, 19], islands [20], etc.

There is a vast literature available on theoretical investigations of spheroidal precipitates/inclusions [21, 22], along with experimental investigations [24–26]. The role of transformation strains on the punching-in of dislocation loops has been studied by Weatherly [27]. For the specific topic of “solutions for spheroidal precipitates in a matrix with different material properties”, the reader may consult Fischer et al. [28]. Investigators have also used alternate computational techniques such as dislocation dynamics to study the coherent to semicoherent transition [29].

The present manuscript is intended to make the following fundamental contributions to our understanding of the coherent to semi-coherent transition of precipitates: (1) model an interfacial edge dislocation loop ascribing separate material properties to the precipitate and the matrix; (2) determine the critical sizes taking into account the interaction between the coherency stresses and dislocation stress fields by: (i) global minimization of energy \( r^* \), (ii) local force balance along the radial direction \( r_2 \) and (iii) local force balance along the circumferential direction \( r_1 \); (3) calcu-
late the stress state of the system (including the precipitate) after critical size has been exceeded (this aspect has been ignored in the standard theoretical approaches [3]); (4) illustrate the power of the methodology developed using a configuration where standard theoretical approaches are inadequate.

A few points to be noted in this regard are listed next. (1) Only the stability along the radial direction has been considered in literature so far (in the current work, we extend the concept of local stability to determine the stable position of the dislocation loop along the circumferential direction). This consideration is important because there is only one global energy minimum, which corresponds to the critical thickness \(r^*\); however, local stability depends on the direction of perturbation (i.e., the loop’s position in the present case). Two natural directions which can be considered are (in accordance with [3]): (i) radial direction (corresponding to \(r_2\)) and (ii) circumferential direction (corresponding to \(r_3\)). In the second case, the loop retains its interfacial character, even when its radius shrinks. Analysis of stability along both these paths is necessary, as it may so happen the loop may be stable with respect to shrinkage along one of these directions, but not along the other (i.e., the loop will not be locally stable). Consideration of local stability is important as it may so happen that during the growth of the precipitate, due to prior history of the sample, an interfacial loop may form for a radius of the precipitate less than \(r^*\). If this happens the loop will be locally stable at the interface. (2) Though the phrase “local force balance” is used to be consistent with literature, the concept of interest is the stability of the dislocation loop at the interface, on the equatorial plane of the precipitate, (3) the detailed treatment of the stability of the dislocation loop, for various diameters of the loop, has not been considered in literature so far and the current work aims to fulfill this shortcoming. This investigation will attempt to validate the methodology, which can be used in future studies to determine critical sizes for precipitation in nanocrystals and effect of other microstructural features on critical sizes.

To this end, the current investigation aims at the following tasks: (1) to develop a finite element model for (a) the precipitation of \(\gamma\)Fe (with 2 wt.% Cu) in the Cu-2 wt.% \(\gamma\)Fe system, (b) an interfacial edge dislocation loop; (2) develop a methodology to compute the critical sizes (\(r^*, r_c\) and \(r_2\)) for coherent to semi-coherent transition, using a combined simulation of a precipitate and an interfacial dislocation loop; (3) determine the stable position of the dislocation loop after critical sizes (\(r^*, r_c\) and \(r_2\)) have been exceeded. The results of the simulations are validated by comparison with available theoretical and experimental results from literature.

2. Theoretical background

The energy of a spherical precipitate of radius “\(r_p\)” in an infinite isotropic matrix is given by [3]:

\[
E_{\text{strain}}^{\text{ppt}} = \frac{8\pi r_p^3 G_{\text{ppt}} (1 + \nu_{\text{ppt}})}{3 (1 - \nu_{\text{ppt}})}
\]  

(1)

Where, “\(G\)” is the shear modulus, “\(\nu\)” is the Poisson’s ratio, \(G_{\text{ppt}}\) is the lattice misfit between precipitate and matrix. The subscript “ppt” refers to the precipitate.

The energy of an edge dislocation loop (\(E_d\)) of radius “\(R\)” is given by [3, 30]:

\[
E_d \approx \frac{G b^2 R}{2(1 - \nu)} \left[ \ln \left( \frac{8R}{c} \right) + 1 \right]
\]  

(2)

Where, “\(b\)” is the modulus of the Burgers vector and ‘\(c\)’ is the core cut-off radius (usually assumed to be in the range of “\(b\)” [30] to 5\(b\) [31]). The core energy is usually about 10% of the total energy [32, 33].

An interfacial misfit edge dislocation loop is a structural defect and is different from a normal edge dislocation loop in the following aspects: (a) the material properties inside and outside the loop are different, (b) the stress fields of the dislocation loop interact with the stress fields of the coherent precipitate and hence are modified (along with the energy of the loop). The first aspect is sometimes accounted for theoretically, by Reuss averaging the material properties of the materials across the interface at which the dislocation is positioned [34]:

\[
G_{\text{average}} = \frac{G_1 G_2}{G_1 + G_2}
\]  

(3)

Where, \(G_1\) and \(G_2\) are the moduli of the two materials. In this simple approach, the entire system is assigned a uniform shear modulus of \(G_{\text{average}}\).

The critical size (\(r^*\)), beyond which an interfacial misfit edge dislocation loop becomes energetically feasible, can be calculated using Eq. (2) for the dislocation loop energy [2, 3, 35]:

\[
r^* = \frac{b}{8\pi \nu (1 - \nu)} \left[ \ln \left( \frac{8r^*}{b} \right) + \frac{3 - 2\nu}{4(1 - \nu)} - 1 \right]
\]  

(4)

Where, “\(\nu\)” (\(\nu = [(1 + \nu) G_m \gamma]/[3(1 - \nu)]\) [36]) is the strain parameter of a constrained system (i.e., of the precipitate). The equation for \(r^*\) (Eq. (4)) is derived based on the criterion that energy released on loop formation is equal to the strain energy of loop (when the precipitate size is \(r^*\)).

Another criterion frequently used is due to Brooks [37]. Brooks had considered an array of interface dislocations, leading to the minimization of strain energy. In the current work we are concerned with the formation of the first interfacial dislocation and hence we keep in focus the work of Brown et al. [2] and Matthews [3].

As discussed before, a precipitate of a lower radius than this (i.e., \(r_c < r^*\)), can also support an interfacial loop due to local force balance (i.e. the line tension force tending to shrink the loop along the radial direction equals the coherence stresses trying to expand the loop); even though, it is not energetically favourable to do so (i.e., if by some means the interfacial loop forms in a precipitate of radius \(r_c\), then it would be stable). This radius (\(r_c\)) is given by [3, 35]:

\[
r_c = \frac{b}{16\pi \nu (1 - \nu)} \left[ \ln \left( \frac{8r_c}{b} \right) + \frac{3 - 2\nu}{4(1 - \nu)} \right]
\]  

(5)

It should be noted that some authors [3, 36] have used the symbols related to critical sizes (\(r^*, r_c\)), with alternate meanings, along with additional symbols relevant to the concept of critical size (\(r_c, r^*\)). In the current work we follow the notation of Brown et al. [2].
3. Finite element methodology

A spherical precipitate of γFe (with 2 wt.% Cu) in a matrix of a solid solution of Cu-2 wt.% Fe, is simulated by imposing stress-free strains (eigenstrains) [38] corresponding to the lattice mismatch strain (misfit strain), between the precipitate and the matrix. Material properties used are [39]:

(i) lattice parameters: \( a_{\text{ppt}} = 3.56 \, \text{Å}, \, a_{\text{matrix}} = 3.61 \, \text{Å} \); (ii) slip system: \(<110>\{111\}; \) (iii) \( b = \sqrt{2} a_{\{110}\}/2 = 2.519 \, \text{Å} \); (iv) \( G\) (ppt) = 88.57 GPa, \( G\) (matrix) = 55.3 GPa; (v) \( v\) (ppt) = 0.2737, \( v\) (matrix) = 0.3234. For anisotropic material properties the following parameters were used: (i) elastic constants: \( C_{11\{pp\}} = 228.92 \, \text{GPa}, \, C_{12\{pp\}} = 134.77 \, \text{GPa}, \, C_{44\{ppt\}} = 116.26 \, \text{GPa}, \, C_{11\{matrix\}} = 170.20 \, \text{GPa}, \, C_{12\{matrix\}} = 122.18 \, \text{GPa}, \, C_{44\{matrix\}} = 76.15 \, \text{GPa}. \) The lattice parameters and the Burgers vector remain the same as those for the case with isotropic material properties. A schematic of the finite element model is shown in Fig. 1 along with the regions (marked as P and D) where stress-free strains are imposed. It should be noted that region-D is a subset of region-P. Inset to the figure shows a 3D view of the precipitate, along with the crystallographic directions. The lattice parameters of the precipitate and matrix are calculated by linear interpolation of lattice parameters; taking the precipitate composition to be Fe-2 wt.% Cu [40] and that of the matrix to be Cu-2 wt.% Fe [41]. Axisymmetry along the \( y\)-axis and boundary conditions imposed, are also illustrated in Fig. 1. The \( y = 0 \) plane is a mirror plane and hence half the domain along the \( y\)-direction is considered in the simulations (to determine \( r^* \) and \( r_c \)). On imposition of the axisymmetry, along with the boundary conditions (as shown schematically in Fig. 1), the precipitate will assume spherical morphology.

The misfit strain (\( \epsilon_m \)) imposed in region-P (Fig. 1) is calculated as: \( \frac{(a_{\text{ppt}} - a_{\text{matrix}})}{a_{\text{ppt}}} = -0.0136 \). The value of \( G \) and \( v \) are calculated by Voigt averaging the data for single crystal elastic constants (\( C_{ij} \)) [32]. The influence of coherency stresses on the lattice misfit strain is neglected. The stress state of a growing precipitate is simulated by increasing the radius of the region-P (Fig. 1), in the finite element model.

The eigenstrain tensor (having only \( \epsilon_{yy} \) component) imposed in region-D (Fig. 1), to simulate an edge dislocation loop is (this strain is given a symbol \( \epsilon_T \), as this is imposed as thermal strains):

\[
\epsilon_T = \frac{1}{2} \left( \frac{a_{\{110\}} + b}{a_{\{110\}} + b} \right) \]

Where, \( a_{\{110\}} (= b) \) is the lattice spacing along the \( \{110\} \) direction of the face centred cubic lattice. The structure and the energy of the core of the dislocation are ignored in the model. Additionally, to be consistent with literature [2 – 4, 35, 41], the dislocation loop considered is a perfect one. It is to be noted that on the introduction of the strain as in Eq. (6), followed by equilibration of the system, most of the domain will be under small strains (except a small region in the vicinity of region-D). As the formulation is based on the assumption of a small strain tensor, in this region in the vicinity of region-D, where the strains are large, the results of the simulation would be inaccurate. This region can be considered as the “core” region of the simulation, akin to the core of a dislocation. To compare the results of the simulation with the theoretical Eq. (2), homogeneous material properties corresponding to that of the matrix is used.

A square domain was meshed with four-noded bilinear plane strain quadrilateral elements, with mesh size \( b \times b \) and stress-free strains were introduced as thermal strains in the numerical model. The model was implemented using the Abaqus/standard (Version 6.81) FEM software. The mesh was refined to \( b \times \frac{b}{2} \) to check for the convergence of the solution on mesh refinement.

A combined model of a growing precipitate and an interfacial misfit loop is used for the determination of the critical size for the presence of the dislocation loop. This is achieved by imposing stress-free strains in regions “P” and “D”, in successive computational steps and calculating the energy of the system after each step. This process is repeated for increasing sizes of the precipitate and the size at which the interfacial dislocation loop becomes energetically favourable (i.e. \( r^* \)), is determined from a plot of energy versus size of the precipitate. To compute \( r^* \), region D is chosen such that the dislocation is positioned at the interface.

To determine the value of “\( r_c \)”, the model in Fig. 1 is extended with three locations of the dislocation loop. Correspondingly, the energy of the loop is determined at three positions: (i) at the interface (at the equatorial plane marked with “S” in Fig. 1), (ii) at \( 1b \) outside the precipitate (+1b)
and (iii) $1b$ inside the precipitate ($-1b$). The gradient of the energy between two successive positions of the dislocation loop (“$b$” apart), gives the driving force experienced by the dislocation loop (the tendency of the force is to expand or shrink the loop). This force acting along the radial direction is given by: $\Delta E_r / \Delta R = \Delta E_r / b$ (where, $E_r$ is the total energy of the system with a coherent precipitate and a dislocation loop as schematically shown in Fig. 1).

If energy is lower at the interface (as compared to $\pm 1b$); then the force is directed towards the interface. It should be noted that this force is different from the force experienced by the interface, which is given by the Eshelby tensor projection normal to the interface as [42]: $f = [\sigma] - <\sigma> [\epsilon]$ (where, $\sigma$ is the stress tensor, $\epsilon$ the strain tensor, $[\cdot]$ means the jump operator and $<\cdot>$ the average operator). For additional theoretical concepts related to the current manuscript, the reader may refer to the book by Abeyaratne and Knowles [42] and Gurtin [43].

To determine the value of $r_i$, the energy of the interfacial loop is determined at two positions: (i) at the equatorial plane (at point “S” in Fig. 1) and (ii) $1b$ below the equatorial plane. The gradient of the energy between these positions is used for the determination of the direction of the force experienced by the loop. For the purpose of calculation of $r_i$, the full domain ($400b \times 800b$) is taken for simulations (other aspects remain the same as before). Additionally, for two sizes of the precipitate (one below $r_i$ and one above $r_i$) the energy of the system for various positions of the loop along the circumferential direction is determined, to understand the nature of the stability of loop.

In a few sample cases anisotropic material properties have been used to illustrate the methodology. This can be extended to other cases as well. It is also assumed that material properties for bulk are valid at the length-scales used in the simulations. It should be noted that the current FEM model being a static model, does not take into account the mechanism of formation of the interfacial dislocation loop (or any of the other kinetic aspects). Additionally, it can only give information on the tendencies based on energetics (e.g. for the dislocation loop to shrink/expand), but cannot determine the actual feasibility.

4. **Validation of the methodology and discussion**

The simulations for only a dislocation loop and only a precipitate are validated first, before the calculation of critical radii. The stress state of the system in the presence of an edge dislocation loop in an axisymmetric domain (i.e. cylindrical domain) is shown in Fig. 2. This is obtained by imposing eigenstrains in region-D (model as in Fig. 1); using material properties corresponding to a homogeneous matrix (i.e. a dislocation loop in Cu-2 wt.% Fe matrix). The energy of the system with increasing radius of the loop is shown in Fig. 3. A good match is seen between the simulated and theoretical plots, within the same order of magnitude. For small loop sizes the domain is expected to behave like an infinite one (as assumed in the derivation of the theoretical equations); increasing the validity of comparison with theory. This also explains the increased deviation with respect to the theoretical curves at larger radii. The plot (Fig. 3) also includes the energy of the dislocation loop calculated with a mesh size of $\frac{b}{2} \times \frac{b}{2}$ (curve labelled C2). A close match between the curves (C1 and C2) is to be noted (the results match to an accuracy less than 1%).

The stress state of the system (plot of $\sigma_{yy}$) on the formation of a spherical precipitate of 40$b$ radius is shown in Fig. 4. The $\gamma$Fe-2 wt.% Cu precipitate has smaller lattice parameter than the Cu-2 wt% Fe matrix. Thus the precipitate is under hydrostatic tension. The strain energy of the system, as computed from the FEM simulations, with an increasing size of the precipitate is shown in Fig. 5. Plots from three simulations are included in the figure: (i) homogeneous and isotropic material properties (corresponding to

![Fig. 2. The stress state of the system (plot of $\sigma_{yy}$ contours) in the presence of an edge dislocation loop of 40$b$ radius. Zoomed-in view shows the region near the dislocation loop.](image-url)

![Fig. 3. Variation in the energy of the system, with an edge dislocation loop of increasing radius. Plot of the theoretical Eq. (2) is also shown for comparison. Good match at lower radii is to be noted. Simulated results with mesh size of $\frac{b}{2} \times \frac{b}{2}$ is also included for comparison (curve labelled C2).](image-url)
the precipitate’s properties), (ii) heterogeneous and isotropic properties, (iii) heterogeneous and anisotropic properties. A comparison with the plot of the theoretical equation is also shown in the figure (Fig. 5a). As expected a good match is seen between the simulated and theoretical values, when homogeneous and isotropic material properties are used in the simulation. Similar to the case of the dislocation loop, the match is better for lower radii, wherein the domain behaves like an infinite one (as assumed in the theoretical Eqs.). The plot (Fig. 5) also includes the energy of the precipitate calculated with a mesh size of $\frac{b}{2} \times \frac{b}{2}$ (curve labelled c2). Akin to the case of mesh refinement for the dislocation loop model, a close match between the curves c1 and c2 is seen (the results match to an accuracy below $10^{-4}$ %).

The modification of the stress state of the system in the presence of an interfacial misfit edge dislocation loop is shown in Fig. 6. It is seen that close to the dislocation loop there is a reversal of the sign of the $\sigma_{yy}$ stress (i.e. the precipitate which was under uniform tension has regions of compression close to the loop). This also implies an increase in energy density (energy per unit volume) of the interfacial region close to the dislocation loop on the formation of the dislocation loop. Due to the interactions of the stress fields of the dislocation with that of the precipitate, there is con-

Fig. 4. Plot of the FEM simulated $\sigma_{yy}$ stress contours in a symmetrical half of the domain, in the presence of a precipitate of radius ($r_p$) = 40b.

Fig. 5. A comparison of the energy of the system as a function of the radius of the precipitate, computed (a) from the theoretical Eq. (1) (b–d) with FEM simulations. It is to be noted that homogeneous, isotropic properties have been used in the theoretical formulation. Simulated result with mesh size of $\frac{b}{2} \times \frac{b}{2}$ is also included for comparison (curve labelled c2).

Fig. 6. FEM simulated $\sigma_{yy}$ stress contours in a domain with a precipitate ($r_p = 50b$) and an interfacial misfit edge dislocation loop. The modification of the stress state in the precipitate is to be noted (in comparison with Fig. 4).
siderable asymmetry between the compressive and tensile stress fields of the dislocation. Within the precipitate the gradient in the dislocation stresses is large (from Fig. 6 it can be seen that the stress values switch from –0.3 GPa to +0.3 GPa within a distance of about 4b).

The energy of the system with an increasing size of precipitate \(r_p\) is shown in Fig. 7: (a) isotropic material proper-
ties and (b) anisotropic properties. The change in energy in the presence of an interfacial misfit edge dislocation loop is also shown in the figure. The point of crossover corresponds to the size of the precipitate at which it becomes energetically favourable to accommodate a misfit dislocation in the system. The critical size \(r^*\) from the plots are: (i) \(\sim 47b\) for isotropic properties and (ii) \(\sim 45b\) for anisotropic properties. For all sizes beyond \(r^*\), the global energy of the system decreases in the presence of the misfit dislocation. Close to the dislocation loop the stress field of the dislocation dominates over the coherency stresses due to the precipitate. This implies that if energy per unit volume is computed close to the loop, the value of this quantity will increase. Interfacial energy \(\gamma\) has been ignored in the current investigation – akin to the previous theoretical models.

Fig. 7. (a) Plot of the total energy of the system, as a function of the size of precipitate \(r_p\), before and after the introduction of an interfacial misfit edge dislocation loop. The point of crossover corresponds to the value of \(r^*\). Simulated result with mesh size of \(\frac{b}{2}\) is also included for comparison (curves labeled with C2). It is to be noted that curves C1 and C2 nearly overlap. Inset (b) shows the corresponding plots with anisotropic material properties in the simulations.

Fig. 8. FEM simulated \(\sigma_{yy}\) stress contours for a domain (model as shown in Fig. 1) having a precipitate of radius \(r_p\) 50b, along with a dislocation loop of radius: (a) 51b (at a distance of “+1b” away from the interface towards matrix region), (b) 49b (at a distance of “−1b” away from the interface in the precipitate region).
Interfacial energy is a constant additive term to the strain energy of the system, as the change in the value of the interfacial energy after the formation of a single misfit dislocation is expected to be small. The figure (Fig. 7) also includes the simulated plots for mesh size $\frac{b}{2} \times \frac{b}{2}$. It is seen that the value of the critical size $r^*$ remains nearly same with a mesh refinement to $b/2$. Based on the above results, in further simulations a mesh size of "$b$" is used.

The results for the determination of $r_c$ are considered in the following discussions. The stress state of the system ($\sigma_{yy}$ plot) for a position of the dislocation loop just off the interface (+1\(b\) and –1\(b\)), is shown in Fig. 8a and b; for a precipitate of 50\(b\) radius (i.e. just beyond \(r^*\)). The important difference between the plot in Fig. 6 (showing an interfacial loop) and Fig. 8a is in the region close to the dislocation loop. For the case of the interfacial loop the stress reversal takes place at the interface; while for the off-interface loop, the stress reversal takes place +1\(b\) from the interface. The inverse of this is true for the loop at –1\(b\) (Fig. 8b). The values of the energy of the system, with increasing radius of the precipitate, determined for loops just off the interface, are listed in Table 1. The table also includes energy values for a dislocation loop located at the interface; along with the direction of the force experienced by the loop, when positioned off the interface. It is seen from the table that for small precipitates the dislocation loop has a tendency to shrink and hence the interface is not a stable position. At a

<table>
<thead>
<tr>
<th>Radius of precipitate (in terms of $b$)</th>
<th>Energy ($\times 10^{-17}$) (J) for dislocation loop positioned at (or from the interface)</th>
<th>Directions of the force experienced by dislocation loop</th>
<th>Comment on the behavior of dislocation loop</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>“–1(b)” (in the precipitate region)</td>
<td>“0” (at the interface)</td>
<td>“+1(b)” (towards the matrix region)</td>
</tr>
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<td>55</td>
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<td>21.699</td>
<td>21.522</td>
</tr>
</tbody>
</table>

Table 1. Comparison of the energy of the system for dislocation loops at the interface and just off the interface (at +1\(b\) and –1\(b\)). The direction of force experienced is shown in the fifth column (the dashed line represents the interface). The length of the vector is approximately representative of the magnitude of the force experienced by the dislocation loop. The terms “shrink” and “expand” refer to tendencies and “r” and “c” refer to radial and circumferential directions.
precipitate size of $\sim 10b$, the energy is minimum for the loop at the interface and hence the interface is a stable position for the loop. Further, it is seen that for the radius of the precipitate between $\sim 10b$ and $\sim 30b$, the interface remains the stable position for the dislocation. Hence, there are three possible ways to arrive at the value of $r_c$ from the results of the simulation: (i) use the least value of $r_p$ at which the interface is a stable position, (ii) use the value of $r_p$ at which there is an force balance, (iii) use the largest value of $r_p$ at which the interface is a stable position. The values of $r_c$ for each of these interpretations are: $\sim 10b$ (25.2 Å), $\sim 13b$ (32.7 Å) and $\sim 25b$ (63.0 Å). According to Brown et al. [2], $r_c$ is the radius of the precipitate at which the force trying to contract the loop ($\partial E_{\text{self}} / \partial r$) is smaller than the interaction force trying to expand the loop ($\partial E_{\text{interaction}} / \partial r$). Using this definition, the value of $r_c$ should be $\sim 25b$ (63.0 Å). However, if we use the definition of $r_c$ by Woolhouse and Ipohorski [35], then force balance should be used as the criterion (i.e. the value of $r_c$ should be taken as $\sim 13b = 32.7$ Å).

Beyond $\sim 30b$ the dislocation will experience a force trying to expand the loop away from the interface and hence the interface is not a stable position for the dislocation loop. To investigate the stable position for the loop, the plot of energy of the system for increasing loop radius (keeping the precipitate radius constant at 50b), is considered as in Fig. 9. It is seen that the energy minimum occurs at 51b, i.e. the loop is stable at $+1b$ from the interface. In fact for precipitate sizes between $\sim 25b$ and $r^*_c$, the stable position of the loop is $+1b$ from the interface. Hence, it is seen that the situation regarding the stability of the loop is more complicated than the picture painted in literature and FEM simulations helps us to explore these aspects.

The value of $r_c$ determined from the simulations is 30b (75.6 Å). If the precipitate size is below 30b, the loop will tend to shrink along the circumferential direction (tending to take it out of the equatorial plane). If the precipitate has a radius larger than 30b the loop will be stable at the equatorial plane along the circumferential direction. Figure 10 shows two plots corresponding to these cases: (a) $r_p (= 10b) < r_c$ and (b) $r_p (= 50b) > r_c$.

The direction of force (along the circumferential direction) for various diameters of the precipitate is summarized in Table 1. It is to be noted that if $r_p$ is in the range $10b \sim 25b$, then the loop will be stable with respect to shrinking in the radial direction but would be unstable along the circumferential direction. For $r_p$ less than 10b the loop is unstable with respect to perturbations in both the directions. Though the kinetic feasibility of these processes is not within the purview of the current simulations, it should be noted that this aspect depends on the temperature, vacancy concentration and other microstructural parameters. The change in the radius of the loop along these two directions (radial and circumferential) has been discussed by Matthews [3] in the context of the formation of the misfit loop.

In the study of epitaxial films, it has been observed that misfit dislocations can have a stable stand-off position from the interface [44]. Freund and Suresh [45] rationalized this in terms of the modulus ratio (modulus of the substrate/modulus of the film). A modulus ratio of at least five is expected to stabilize the misfit dislocation off the interface (in the film). In the case of semi-coherent precipitate systems, we note that a modulus ratio of just $\sim 1.5$ can stabilize the loop off the interface (this aspect can be thought of arising from the spherical geometry of the precipitate).

Watanabe et al. [41] have experimentally determined the critical size ($r_c^*$) of precipitates in the Cu-2 wt.% Fe system to be about 100 Å. They have shown that the precipitate is coherent below 100 Å and becomes incoherent when the size of the precipitate exceeds 200 Å. Earlier investigations [40, 46] have reported precipitate size values for incoherent precipitates to be in the range of 250 –300 Å. In the current work we use the results of Watanabe et al. [41] (for validation), as their reported value corresponds to the transition from coherent to semi-coherent state; while the results of the earlier experimental investigations are for incoherent precipitates.

Table 2 gives a comparison of the critical size values obtained from FEM simulations, with theoretical results [2, 3] and experimental observations [41]. A good match is seen for the $r^*_c$ value computed using the FEM model, with experimental observations and theoretical calculations. This on the one hand is to be expected, as the “essential physics” underlying the computations are the same; while, on the other hand the assumptions underlying the models are different and hence a perfect match is not to be expected. Sep-

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**Fig. 9.** The variation in the energy of a system (FEM results), for dislocation loops of increasing radii. The precipitate radius is kept constant at 50b. The energy minimum is at 51b.

**Fig. 10.** The strain energy of an interfacial loop as a function of its position from the equatorial plane ($\gamma$): (a) $r_p = 10b$, (b) $r_p = 50b$.
arate material properties have been used for the precipitate and matrix in the FEM model, while the theoretical model assumes uniform material properties. In the FEM model there is a “core” region (about two elements wide and half the domain in height), where the strains are large (with corresponding errors introduced due to this); while in the theoretical equation there is no “core” with respect to stresses. In the simulations finite domains have been used, while in the theoretical model, domains are assumed to be infinite. Additionally, as domain has been discretized by $b \times b$ mesh elements, all the computed results suffer similar discretization and approximation. An important point to be noted from Table 2 is that for no size of the precipitate is the loop stable along both the radial and circumferential directions (at point “S” in Fig. 1). Hence, even when the loop becomes energetically feasible (by global energy minimization), it is not locally stable at point “S”. However, for $r_p > r^*$, the loop is stable at +1$b$ from the interface, along the radial direction.

Regarding the comparison of $r_c$ value determined from simulation with theoretical results, only the upper limit of $r_c$ determined from finite element simulations matches well with the theoretical results. The reason for this is as discussed before.

Jesser [36] using a value of Burgers vector corresponding to that of pure $\gamma$Fe, has calculated a value of $r^*$ to be 108 Å. In the current investigation the precipitate composition is to be Fe-2 wt.% Cu, in accordance with the phase diagram [40].

The foregoing discussions highlight the following advantages of the current methodology: (i) separate material properties have been used for the precipitate and the matrix; (ii) the stress state of the system is determined after critical size has been exceeded; (iii) equilibrium position of the loop (including stand-off if any) can be computed. Additionally, the current work can readily be extended to compute critical sizes for the feasibility of multiple interfacial dislocation loops and the effect of presence of other precipitates and dislocations in the domain on the critical sizes.

5. Example to illustrate the utility of the methodology

In this section the power and utility of the methodology developed in the current work is illustrated by considering the model shown in Fig. 11. This represents a spherical precipitate in a domain in the shape of a thin disc. The thickness of the domain is 403 Å. This case corresponds to a configuration where standard theoretical equations are not available and theoretical analysis would be extremely cumbersome (the reasons for the same are considered along with the results in the next paragraph).

Using the methodology developed in the preceding sections, the critical thicknesses are determined. The values for the model in Fig. 11 are: (i) $r^* = 57b$ (143.6 Å), $r_c = 13b$ (32.7 Å) and $r_t = 30b$ (75.6 Å). It is seen that the $r^*$ value is altered with respect to the large domain considered before (which can be thought of as a “bulk domain”); while $r_c$ and $r_t$ values are same as that for the bulk domain. This alteration is due to two effects: (i) reduction in the strain energy of the precipitate (due to lesser volume of strained material), (ii) relaxation of strain energy due to domain deformations. The strain energy of the precipitate of radius ($r_p$) of 60Å for a “bulk” domain is $5.46 \times 10^{-16}$ J, while for the thin disc the value is $5.19 \times 10^{-16}$ J. The second aspect (domain deformation) is shown in Fig. 12. It is

![Fig. 11. Schematic of the FEM model used for the simulation of a precipitate (without and with a dislocation loop) in a thin disc (with thickness of 160b). The crystallographic orientation is identical to that in Fig. 1.](image1)

![Fig. 12. Stress state (FEM simulated $\sigma_{xx}$ stress contours) on precipitation in a thin disc (model as in Fig. 10). The radius of the spherical precipitate is 60b. Deformation scale factor is 6. Inset shows the region near the precipitate, highlighting the domain deformation (scale factor is 10 for inset and attention is to be paid to the region marked with an ellipse).](image2)
to be noted that the energy of the dislocation loop in the finite domain will also be reduced with respect to its value in a “bulk domain”; but as the precipitate energy has a stronger dependence on the radius, the truncation of the domain (crystal) would affect (i.e. reduce) the strain energy of the precipitate more than that of the dislocation loop. The reason that \( r_c \) and \( r_f \) values remain unaltered is that, only when the precipitate diameter is a considerable fraction of the thickness of the disc, does the “finiteness” of the domain become important.

6. Summary and conclusions

The stress state of a growing precipitate, without and with an interfacial misfit dislocation loop, is simulated by imposing stress-free strains in appropriate region(s) of a finite element model. A methodology is developed to determine the critical size of the precipitate (\( r^* \)), at which a misfit edge dislocation loop becomes energetically feasible. The model is extended to calculate the value of the radius at which a dislocation loop can be stable at the interface (\( r_c \)) against shrinkage in the radial direction. Further, a new concept of the stability of the dislocation loop along the circumferential direction is introduced and the critical size (\( r_c \)) at which the loop is stable at the equatorial plane is determined using the FEM model. The Cu-\( \gamma \)Fe alloy is considered as a model system for the simulations. The methodology developed is validated by a comparison of the values calculated from the model, with available experimental and theoretical results. It is seen that for precipitate sizes greater than \( r > 30b \) the dislocation is stable off the interface (at \( +1b \) along the radial direction). The FEM simulations reveal that the situation regarding the stability of the dislocation loop is considerably more involved than the picture presented in literature till now (force balance vis-à-vis force directed towards the interface is differentiated in this context). It is seen that for no size of the precipitate is the loop stable at the interface, along both the radial and circumferential directions. Use of anisotropic material properties does not influence the value of critical thickness in a significant way. Further, an example of precipitation in a thin disc is considered to illustrate the power of the methodology for the determination of critical sizes (\( r^*, r_c \) and \( r_f \)) in situations, where standard theoretical equations are not available and analytical formulations would be cumbersome. It is seen that in a thin disc the value of \( r^* \) is increased with respect to that for a “bulk domain”. The methodology developed can be extended to complex configurations such as: (a) presence of multiple precipitates of various sizes and distributions, multiple matrix materials, other dislocations etc.; (b) complex precipitate geometries; (c) precipitation in nanomaterials (i.e. the matrix is confined in one, two or three dimensions); (d) precipitation in epitaxial films.

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