



University of Pennsylvania  
ScholarlyCommons

---

Departmental Papers (MSE)

Department of Materials Science & Engineering

---

November 2000

# Strain-Rate Dependence of the Brittle-to-Ductile Transition Temperature in TiAl

Mahadevan Khantha

*University of Pennsylvania*, [khantha@seas.upenn.edu](mailto:khantha@seas.upenn.edu)

Vaclav Vitek

*University of Pennsylvania*, [vitek@lrsm.upenn.edu](mailto:vitek@lrsm.upenn.edu)

David P. Pope

*University of Pennsylvania*, [pope@seas.upenn.edu](mailto:pope@seas.upenn.edu)

Follow this and additional works at: [http://repository.upenn.edu/mse\\_papers](http://repository.upenn.edu/mse_papers)

---

## Recommended Citation

Khantha, M., Vitek, V., & Pope, D. P. (2000). Strain-Rate Dependence of the Brittle-to-Ductile Transition Temperature in TiAl. Retrieved from [http://repository.upenn.edu/mse\\_papers/11](http://repository.upenn.edu/mse_papers/11)

Copyright Materials Research Society. Reprinted from MRS Proceedings Volume 646.

2000 Fall Meeting Symposium N

High-Temperature Ordered Intermetallic Alloys IX

Publisher URL: [http://www.mrs.org/members/proceedings/fall2000/n/N1\\_11.pdf](http://www.mrs.org/members/proceedings/fall2000/n/N1_11.pdf)

This paper is posted at ScholarlyCommons. [http://repository.upenn.edu/mse\\_papers/11](http://repository.upenn.edu/mse_papers/11)

For more information, please contact [libraryrepository@pobox.upenn.edu](mailto:libraryrepository@pobox.upenn.edu).

---

# Strain-Rate Dependence of the Brittle-to-Ductile Transition Temperature in TiAl

## **Abstract**

The brittle-to-ductile transition (BDT) and the strain-rate dependence of the brittle-to-ductile transition temperature (BDTT) have been recently investigated in single crystals of TiAl [1]. It was found that the activation energy associated with the BDTT is 1.4 eV when the slip is dominated by ordinary dislocations and 4.9 eV when it is dominated by superdislocations. Despite this difference in the activation energies, the BDTT, while varying with the strain-rate, remains in the same temperature range, viz., between 516-750C and 635-685C for ordinary and superdislocations, respectively. In this paper, we examine how the activation energy of the BDTT can vary with the type of dislocation activity and explain why it can attain values which are clearly much larger than the activation energy for dislocation motion. We describe a strain-rate dependent mechanism of cooperative dislocation generation in loaded solids above a critical temperature and use it to explain the characteristics of the BDT in TiAl. We show that the activation energy associated with the BDTT is a composite value determined by two or more inter-dependent thermally activated processes and its magnitude can be much larger than the activation energy for dislocation motion in certain materials. The predictions of the model are in good agreement with observations in TiAl.

## **Comments**

Copyright Materials Research Society. Reprinted from MRS Proceedings Volume 646.

2000 Fall Meeting Symposium N

High-Temperature Ordered Intermetallic Alloys IX

Publisher URL: [http://www.mrs.org/members/proceedings/fall2000/n/N1\\_11.pdf](http://www.mrs.org/members/proceedings/fall2000/n/N1_11.pdf)

## STRAIN-RATE DEPENDENCE OF THE BRITTLE-TO-DUCTILE TRANSITION TEMPERATURE IN TiAl

M. Khantha, V. Vitek and D. P. Pope  
Department of Materials Science and Engineering, University of Pennsylvania,  
Philadelphia, PA 19104-6272

### ABSTRACT

The brittle-to-ductile transition (BDT) and the strain-rate dependence of the brittle-to-ductile transition temperature (BDTT) have been recently investigated in single crystals of TiAl [1]. It was found that the activation energy associated with the BDTT is 1.4 eV when the slip is dominated by ordinary dislocations and 4.9 eV when it is dominated by superdislocations. Despite this difference in the activation energies, the BDTT, while varying with the strain-rate, remains in the same temperature range, viz., between 516-750C and 635-685C for ordinary and superdislocations, respectively. In this paper, we examine how the activation energy of the BDTT can vary with the type of dislocation activity and explain why it can attain values which are clearly much larger than the activation energy for dislocation motion. We describe a strain-rate dependent mechanism of cooperative dislocation generation in loaded solids above a critical temperature and use it to explain the characteristics of the BDT in TiAl. We show that the activation energy associated with the BDTT is a composite value determined by two or more inter-dependent thermally activated processes and its magnitude can be much larger than the activation energy for dislocation motion in certain materials. The predictions of the model are in good agreement with observations in TiAl.

### INTRODUCTION

The brittle-to-ductile transition (BDT) exhibited by most crystalline materials is a strain-rate dependent phenomenon marked by a rapid increase of dislocation activity at the crack tip concomitant with a sharp increase of the fracture toughness [2, 3]. The brittle-to-ductile transition temperature (BDTT) increases with increasing strain-rate in all materials and an apparent activation energy can be associated with this strain-rate dependence. In silicon and other semiconductors [2, 3], this activation energy is almost exactly equal to the activation energy for dislocation motion. It is not known if such a correlation exists in other classes of materials.

The BDT in TiAl single crystals [1] was recently investigated for two different crack geometries. It was found that the activation energy associated with the BDTT is 1.4 eV when the slip is dominated by ordinary dislocations (Burgers vector  $1/2\langle 110 \rangle$ ) and 4.9 eV when it is dominated by superdislocations (Burgers vector  $\langle 011 \rangle$ ). Despite this difference in the activation energies, the BDTT, while varying with the strain rate, is in the same temperature range, viz., between 516-750C and 635-685C for ordinary and superdislocations, respectively [1]. In addition, the variation of the fracture toughness with temperature was identical for both geometries over the entire temperature range for a fixed strain-rate. This suggests that the activation energy for motion of ordinary dislocations and superdislocations must be similar. The activation energy for dislocation motion is not known in TiAl but there is considerable evidence which suggests that the activation energy for the glide of ordinary dislocations is only slightly lower than that for superdislocations [4, 5]. In both cases, the activation energy is not expected to be as high as in Si (1.8-2.2 eV) because both types of dislocations are known to glide at low temperatures. This raises the question why the apparent activation energy of the BDTT is significantly different for ordinary and superdislocations when this difference cannot be sought in different mobilities of these two types of dislocations.

We describe a strain-rate dependent process of cooperative dislocation generation in loaded crystals that can lead to the formation and expansion of many dislocation loops without any energy barrier above a critical temperature [6-9]. In particular, the model shows that the apparent activation energy associated with the BDTT represents a composite phenomena of two or more inter-dependent thermally activated processes. Its value is determined not only by the activation energy for dislocation motion but also by the density of glissile dislocations. The latter includes pre-existing mobile dislocations and dislocations that are precursors to the onset of the cooperative instability, generated just below the BDTT, by thermal activations. In this paper we use this model to explain the BDT and predict the BDTT in TiAl for activity of both ordinary and superdislocations. We show that small changes in the density of pre-existing glissile dislocations (ordinary or superdislocations) can result in large changes in the apparent activation energy associated with the BDTT without affecting the magnitude of the BDTT significantly. The results are in good agreement with observations.

## STRAIN-RATE DEPENDENT COOPERATIVE PROCESS OF DISLOCATION GENERATION

The cooperative dislocation generation proceeds by the concurrent nucleation and evolution of many atomic-size dislocation loops that form in a loaded crystal at finite temperatures. This process, which occurs owing to the combined effect of dislocation interactions and entropy [6-9], differs manifestly from the nucleation and subsequent expansion of an isolated dislocation loop [10]. At finite temperatures, in a loaded crystal, there is a small probability of forming dislocation loops of interatomic dimensions by thermal fluctuations since their energy ranges approximately from 1.0 - 2.0 eV. The density of such loops of radius  $r$  at temperature  $T$  is determined by the Boltzmann factor,  $\exp[-H(r)/k_B T]$ , where  $H(r)$  is the formation enthalpy of the loop and  $k_B$ , the Boltzmann constant. For an isolated shear loop [8], when the material is loaded by a shear stress  $\sigma$  in the direction of the Burgers vector,

$$H(r) = K_0 [r \ln(r/r_0) + cr] - \sigma b \pi r^2 \quad (1)$$

where  $K_0 = [\mu_0 (2 - \nu_0) b^2 / 4(1 - \nu_0)]$ ,  $b$  is the magnitude of the Burgers vector,  $\mu_0$  the elastic shear modulus in the slip plane,  $\nu_0$  the Poisson ratio,  $K_0 c$  the core energy of the dislocation and  $r_0$  the elastic cut-off radius. Dislocation loops formed by thermal fluctuations mostly shrink and disappear because their radii are considerably smaller than the critical radius ( $\sim$  ten lattice spacing) at which  $H(r)$  reaches a maximum ( $\sim$  10 eV) for applied stresses appreciably smaller than the ideal shear strength of the material. Hence, the homogeneous nucleation of dislocations has always been regarded as highly improbable [11]. The cooperative generation of dislocations is entirely different.

The fundamental principle underlying this process is the recognition that interactions between dislocation loops, even when they are of atomic-sizes, can lead to changes in the dislocation configuration whereby some loops expand while others shrink in order to minimize their total energy. Thus, when a dislocation loop is formed in a loaded crystal containing other dislocation loops, the re-arrangement of the existing loops under the stress field of the newly formed loop is associated with an incremental *net plastic strain*. A straightforward way to investigate the effect of dislocation interactions is to examine how the incremental plastic strain can influence the subsequent nucleation of dislocations in the loaded crystal [7]. Here, we are guided by the well-known result that dislocation glide resulting in net plastic strain is associated with a decrement of the effective modulus that relates stresses and total strains in the crystal [11]. The reduction of the effective moduli due to interactions between atomic-size dislocation loops is usually many orders of magnitude smaller than the typical 10-20% reduction observed for high densities of mobile dislocations. Nevertheless, even this small reduction of the effective moduli can have a spectacular effect on the nucleation and interaction of subsequent dislocations as a function of increasing temperature. This is a consequence of a complex

feedback process which couples the modulus decrement to the density of thermally nucleated dislocations while their interactions determine the magnitude of the decrement. Thus, even a very small decrement in the effective modulus results initially in a small but exponential increase in the density of thermally nucleated dislocations. The enhanced density leads to increased interactions and hence a slightly larger decrement of the modulus along with a greater increase in the density of loops. This feedback process is accentuated as temperature increases at a fixed applied load until it leads to an instability as explained below.

The self energy of a newly formed dislocation loop in a crystal containing other loops is proportional to a combination of effective moduli just as the energy of an isolated dislocation loop is proportional to a combination of elastic moduli. Thus, the formation enthalpy of a loop in a medium containing other loops can be written as in equation (1) but with  $K_0$  replaced by  $K_{\text{eff}} = K_0/\epsilon$ , where  $\epsilon$ , called a 'screening function', is akin to a 'dielectric function' and  $K_{\text{eff}}$  is the energy coefficient written in terms of the effective moduli.  $\epsilon$  reflects the decrease of the self energy of a dislocation loop due to the interactions between other loops. At low temperatures, the difference between the effective and elastic moduli is very small and  $\epsilon$  is nearly equal to unity which is its minimum value. As the temperature increases, the probability of formation of dislocation loops in a loaded crystal increases which in turn, increases the plastic strain in the medium. Consequently, the effective moduli decrease and  $\epsilon$  increases slowly from its baseline value of unity. As a result, the formation enthalpy of a loop present amidst other dislocation loops is smaller than that of an isolated loop of the same size. This, in turn, promotes the formation of more dislocation loops in the crystal which further increases the plastic strain. A positive or 'cooperative' feedback is set up between the formation of additional sub-critical dislocation loops and the continued reduction of the effective moduli.

Concomitant with the reduction of the formation energy, the critical radius for expansion of the loop and the related activation enthalpy decrease progressively as the temperature increases [8, 12]. (In contrast, the barrier for the expansion of a single dislocation loop does not vary with temperature.) At the same time, the configuration entropy associated with the dislocation loops increases as their number increases with temperature. Ultimately, at a critical temperature,  $T_c$ , the free energy of the loops vanishes. The unstable expansion and glide of the loops above  $T_c$  implies that spontaneous nucleation and glide of many dislocation loops can occur in the stressed crystal. The ensuing massive dislocation activity makes the effective moduli approach zero or, equivalently,  $\epsilon$  diverge to infinity above  $T_c$  while the value of  $\epsilon$  at  $T_c$  remains finite. For large applied loads, of the order of  $\mu_0/100$ , the critical temperature is typically half of the melting temperature [8].

The static model, described above, treats a dislocation-free crystal and examines how collective generation of glissile dislocations becomes feasible above a certain temperature under large applied loads. We now consider two types of dislocation activity which can significantly affect the onset of this instability. First, the glide of pre-existing mobile dislocations below  $T_c$  contributes to the plastic strain similarly as the formation of sub-critical dislocation loops does in the static model [7]. Hence, this additional plastic strain is expected to aid the cooperative instability and bring about a lowering of the critical temperature. Second, with increasing temperature, dislocation interactions lower the activation barrier for the cooperative generation of dislocations significantly. The barrier falls below 2 eV typically in the range 100-200K below  $T_c$ , thus enabling the generation of glissile dislocations by thermal activation in this temperature regime [8, 12]. The glide of such 'thermally nucleated' dislocations contributes to the plastic strain similarly as the glide of pre-existing dislocations and leads to further lowering of the critical temperature.

For a given set of material parameters and fixed external loads, the cooperative instability commences at a critical temperature when  $\epsilon$  attains a critical value,  $\epsilon_c$ . (The magnitude of  $\epsilon_c$  is typically in the range 1.0 - 1.5 for most materials.) The glide of pre-existing dislocations causes the initial modulus decrement which then influences the nucleation of sub-critical dislocation loops and lowers the activation barrier for collective expansion of the loops. In a 100-200K interval below the critical temperature, thermally nucleated dislocations can also glide

macroscopically and this in turn affects the nucleation of sub-critical dislocation loops and the onset of the cooperative instability. It is ultimately the expansion of sub-critical loops which occurs when the free energy becomes zero that triggers the cooperative instability. The macroscopic glide of dislocations is always strain-rate dependent, and thus, the BDTT predicted by this model [9] is also strain-rate dependent.

In a previous paper, it was shown [13] that the dislocation dynamics in the vicinity of cracks is of "similarity" type when the velocity of dislocations is a power law function of the stress with exponent  $m$  and the motion is thermally activated with activation barrier  $U_m$ . At the BDTT the density of thermally nucleated dislocations,  $n_f$  is proportional to  $\exp(-U_n/k_B T_c)$  where  $U_n$  is an apparent formation energy and  $T_c$  refers to the strain-rate dependent BDTT [9]. Using this analytical form it can be shown [9] that the apparent activation energy,  $U_{app}$ , associated with the strain-rate dependence of the BDTT is given by

$$U_{app} = U_m + ((m + 2)/2(m + 1))U_n \quad (2)$$

The formation energy,  $U_n$ , is however, not a constant. It is temperature-dependent and its value depends on how effectively the glide of pre-existing dislocations lowers the formation energy for cooperative generation of dislocations. Depending on the density of pre-existing dislocations and their mobility, the apparent activation energy associated with the strain-rate dependence of the BDTT is predicted to be either equal to or larger than the activation energy for dislocation motion.

## RESULTS AND DISCUSSION: APPLICATION TO TiAl

According to our model, the glide of pre-existing dislocations and dislocations thermally nucleated below the BDTT, gives rise to the strain-rate dependence of the BDTT. The model also shows that the apparent activation energy associated with the BDTT,  $U_{app}$ , is not connected with a well-defined activation process. Rather, it is determined by the combined interplay between the nucleation of dislocations at BDTT and the motion of pre-existing and newly formed dislocations. The density of pre-existing dislocations,  $n_0$ , can influence the apparent formation energy of thermally nucleated dislocations below the BDTT and this can cause  $U_{app}$  to be bigger than the activation energy for dislocation motion,  $U_m$  (see Equation 2). We now examine how  $U_{app}$  varies in TiAl with changes in  $n_0$  and the type of dislocation activity.

Table 1. Model predictions for the strain-rate dependence of the BDTT in TiAl

Dislocation type	Initial dislocation density $n_0$ ( $m^{-2}$ )	BDTT (K) for strain rates $10^{-5}$ , $10^{-4}$ , and $10^{-3} \text{ sec}^{-1}$	$U_m$ (eV)	$U_{app}$ (eV)
1/2<110]	$10^8$	763, 800, 820	1.0	4.9
1/2<110]	$10^{10}$	672, 746, 807	1.0	1.6
<011]	$10^8$	926, 962, 974	1.2	6.8
<011]	$10^{10}$	808, 896, 960	1.2	2.0
<011]	$10^{12}$	929, 976, 999	2.0	5.0
<011]	$10^{14}$	841, 903, 970	2.0	2.5

The parameters that determine the BDTT in our model include the shear modulus on the slip plane, Burgers vector, applied stress, dislocation core energy, elastic cut-off radius, velocity-

stress exponent,  $m$ , the activation barrier for dislocation motion,  $U_m$ , and two constants related to the dislocation mobility and the similarity solution, respectively<sup>1</sup>. We set the activation energy for dislocation motion,  $U_m$ , for ordinary dislocations to a low value of 1 eV. In the case of superdislocations, we investigate how the BDTT varies for two different values of the activation energy for dislocation motion. In the first case, a value slightly higher than that for ordinary dislocations is assumed, namely  $U_m = 1.2$  eV, consistent with observations. In the second case, a much higher value is chosen, namely,  $U_m = 2.0$  eV. This value is close to the activation energy for motion of dislocations in Si. The velocity-stress exponent  $m$  is set equal to unity and the BDTT is calculated for strain rates in the range  $10^{-5}$  to  $10^{-3}$  sec<sup>-1</sup>. The variation of the BDTT with the density and type of dislocation activity is shown in Table 1.

We find that the apparent activation energy associated with the BDTT can change dramatically for two orders of magnitude change in the density of pre-existing dislocations in TiAl, irrespective of the nature of dislocation activity. This is especially apparent when the activation energy for dislocation motion has a low value such as 1.0-1.2 eV. The reason for this is as follows: When the activation energy for dislocation motion is small, the modulus decrement from the glide of pre-existing dislocations makes a significant contribution to  $\epsilon$  when the density,  $n_0$ , is large. This leads to a significant reduction of the apparent formation energy for thermally nucleated dislocations ( $U_n$ ), and thus  $U_{app}$  (see Equation 2) which then results in lowering of the BDTT. Interestingly, the calculated values of the BDTT lie in the same range for the two densities despite the significant difference in  $U_{app}$  for ordinary and superdislocation activity. A higher value of  $U_{app}$  necessarily corresponds to a higher BDTT at low strain-rates but this trend becomes unnoticeable at higher strain-rates. This follows from the fact that at higher strain-rates, the time available for dislocation glide before fracture occurs is very small. Therefore, the contribution to  $\epsilon$  from the glide of pre-existing and thermally nucleated dislocations becomes very small and the onset of the cooperative instability is almost entirely controlled by the nucleation of sub-critical dislocation loops albeit at higher temperatures. It is this feature which leads to considerable overlap in the range of the BDTT for two widely different values of  $U_{app}$ .

Let us consider the case where the activation energy for superdislocation motion is set to 2.0 eV, a value close to that for dislocation motion in Si. The model predicts that  $U_{app}$  again varies appreciably with the initial density of glissile dislocations. However, compared to smaller values of  $U_m$ , the value of  $U_{app}$  is only 25% larger than the activation energy for motion when the mobile dislocation density is high. It is interesting to compare this trend for TiAl with that for Si for a similar value of  $U_m$ . Experiments in Si [2, 14, 15] indicate that  $U_{app} \sim U_m$ . It is also known that the initial density of glissile dislocations is very low in most experiments. These observations, at first, seem to contradict the trend seen in TiAl for the case of  $U_m = 2.0$  eV. However, in order to perform a meaningful comparison we calculated the strain-rate dependence of the BDTT in Si using the parameters appropriate to this material<sup>2</sup>. We varied the initial mobile density ( $n_0$ ) from a low value of  $10^6$  m<sup>-2</sup> to  $10^{10}$  m<sup>-2</sup>. We found,  $U_{app} = 2.2$  eV for

<sup>1</sup> The Burgers vector is set as  $b = 2.83$  Å for ordinary dislocations and  $b = 5.7$  Å for superdislocations in TiAl.  $\mu_0 = 70$  GPa and  $\nu_0 = 0.23$  represent average values for polycrystalline TiAl; the cut-off radius,  $r_0$ , is set equal to the appropriate Burgers vector in the two cases; the core energy factor  $c = 0.25$  for ordinary dislocations and  $c = 0.23$  for superdislocations. We assume the material to be loaded by a constant large stress,  $\sigma = 3$  GPa for both types of dislocation activity. Such stress levels are expected in the vicinity of a crack. In addition to these parameters, two new constants enter the analysis: (i) The time available for dislocation glide at a certain strain-rate before fracture takes place which is estimated from experimental data [1]; and (ii) the constant appearing in the 'similarity' solution for dislocation motion near crack tips [13] which is chosen such that the BDTT lies in a reasonable range.

<sup>2</sup> For Si  $b = 2.21$  Å corresponding to  $1/6\langle 112 \rangle$  Shockley partial dislocation,  $\mu_0 = 60.5$  GPa (the shear modulus on the (111) plane),  $\nu_0 = 0.22$ ,  $r_0 = 3.83$  Å (the nearest-neighbor spacing),  $c = 0.53$  such that the formation enthalpy of an isolated loop of radius  $5$  Å is approximately 1eV and  $m = 1$ . The stress was assumed to be the same as in TiAl, namely,  $\sigma = 3$  GPa. The activation energy for dislocation motion,  $U_m$ , was set equal to 2.1 eV.

$n_0 = 10^{10} \text{ m}^{-2}$  and  $U_{\text{app}} = 2.6 \text{ eV}$  for  $n_0 = 10^6 \text{ m}^{-2}$ . Thus,  $U_{\text{app}}$  is quite close to  $U_m$  (2.1 eV) and does not depend sensitively on the density of pre-existing dislocations. While this is in good agreement with experiments in Si [2, 14, 15], it is different from the trend obtained for TiAl. The reason  $U_{\text{app}}$  varies appreciably in TiAl even for large values of  $U_m$  unlike the case in Si is related to a number of factors. In addition to the density of pre-existing dislocations, other parameters which can also raise or lower the values of  $U_n$  and hence,  $U_{\text{app}}$ , are the Burgers vector, the shear modulus and dislocation core energy. All these quantities are different for superdislocations in TiAl compared with the values used for partial dislocations in Si. Thus, in addition to the activation energy for dislocation motion and the density of pre-existing mobile dislocations, other material parameters also influence  $U_n$  and hence,  $U_{\text{app}}$ . Summarizing the model predictions, we find that the most plausible explanation for the large difference in  $U_{\text{app}}$  between ordinary and superlattice dislocation activity in TiAl observed by Booth and Roberts [1] is that the initial mobile densities of the two types of dislocations are significantly different but their mobilities are not vastly different.

In conclusion, a cooperative mechanism of dislocation generation above a critical temperature can give rise to massive dislocation activity of the type associated with the BDT. The strain-rate dependence of the critical temperature arises from the motion of pre-existing dislocations and dislocations which are "thermally nucleated" below the critical temperature by the cooperative process. The corresponding activation energy is not associated with one unique thermally activated process (such as dislocation motion) but represents an apparent value similarly as the activation energy associated with diffusion coefficients. This dependence is more complex in the case of BDTT than in diffusion because two or more thermally activated processes related to dislocation nucleation and glide are coupled together. Depending on their contributions, the apparent activation energy associated with the BDTT is either equal to or larger than the activation energy for dislocation motion.

## ACKNOWLEDGMENT

This research was supported by the US Air Force Office of Scientific Research grant F49620-98-1-0245.

## REFERENCES

1. A. S. Booth and S. G. Roberts, *Acta Mat.* **45**, 1045 (1997).
2. C. St. John, *Philos. Mag.* **32**, 1193 (1975).
3. S. G. Roberts, A. S. Booth and P. B. Hirsch, *Mat. Sci. & Eng.* **A176**, 91 (1994).
4. K. Kishida, H. Inui and M. Yamaguchi, *Phil. Mag. A* **78**, 1 (1998).
5. M.-C. Kim, M. Nomura, V. Vitek and D. P. Pope, *High-Temperature Ordered Intermetallic Alloys VIII* (edited by E. George, M. Mills and M. Yamaguchi), Materials Research Society, Vol. 552, p. KK3.1.1 (1999).
6. M. Khantha, D. P. Pope and V. Vitek, *Phys. Rev. Lett.* **73**, 684 (1994).
7. M. Khantha and V. Vitek, *Acta Mater.* **45**, 4675 (1997).
8. M. Khantha and V. Vitek, *Mat. Sci. & Eng.* **A234-236**, 629 (1997).
9. M. Khantha, V. Vitek and D. P. Pope, *Mat. Sci. & Eng. A* to appear, (2000).
10. J. R. Rice and R. Thomson, *Philos. Mag.* **29**, 73 (1974).
11. F. R. N. Nabarro, *Theory of Crystal Dislocations*, Dover: New York (1967).
12. M. Khantha, M. Ling and V. Vitek, *Mat. Sci. Res. Int.* **5**, 234 (1999).
13. M. Khantha, *Scr. Metall. Mater.* **31**, 1355 (1994).
14. M. Brede and P. Haasen, *Acta Metall.* **36**, 2003 (1988).
15. J. Samuels and S. G. Roberts, *Proc. R. Soc. Lond.* **A 421**, 1 (1989).