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Dissociation of $a<100>$ edge superdislocations in the γ' -phase of nickel-base superalloys

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Abstract

Dissociation of $a<100>$ edge superdislocations in Ni_3Al , the hardening γ' -phase of nickel-base superalloys, was investigated using molecular dynamics simulations and theory of elasticity. It was shown that these dislocations dissociate either symmetrically or asymmetrically when they are close to the $<011>$ orientation. The symmetric dissociation, called Hirth lock, has the lowest energy. The reasons for the dissociation are the strong energy reduction due to the core splitting and the relaxation of elastic strains within the dissociation area. The dissociation of $a<100>$ edge superdislocations is the reason for their alignment in $<011>$ orientation in the γ' -rafts of superalloys. However, the dissociation does not block the movement of the dislocation because they penetrate the γ' -rafts by climbing. Under loading conditions, typical for creep tests of nickel-base superalloys at high temperatures ($\geq 1000^\circ\text{C}$), the Hirth lock slightly expands but remains stable. The asymmetric configuration is less stable and can transform into the lower energy Hirth lock.

1. Introduction

Nickel-base superalloys are used for the blades of gas turbines operating at temperatures up to 1100°C for thousands of hours. These high temperature materials have a two phase microstructure: the matrix is a γ -solid solution of nickel (structure type A1), which is strengthened by small precipitates of the γ' -phase (ordered structure of type L_{12} on the base Ni_3Al). One reason for the excellent mechanical properties of superalloys is the Kear-Wilsdorf locking mechanism, established by these scientists for Cu_3Au [1] and then introduced by Copley and Kear [2] for Ni_3Al : $a<110>$ superdislocations, typical for the L_{12} structure, dissociate at high temperatures in a characteristic nonplanar manner, reducing the dislocation mobility.

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Recently it was reported that at high temperatures (around 1100°C) and low stresses a different kind of superdislocation penetrates the γ' -phase, namely $a<100>$ dislocations [3,4]. With this new kind of a superdislocation the question immediately arose, how it moves under high temperature conditions? A prerequisite for such a discussion is the knowledge of the core structure of the $a<100>$ superdislocation.

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$a<100>$ dislocations were first found in single phase Ni_3Al by Veyssire and Douin [5]. This result was confirmed by Sun and Hazzeldine [6]. Additionally it was found, that these dislocations preferably have $<110>$ line directions, forming an angle of 45° with the Burgers vector $\bar{b}$. So $a<100>$ dislocations are gliding on $\{001\}$ planes and distinctly become pinned, when the line vector attains $<110>$ orientation. It was proposed that the pinning mechanism is a so

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called B5 lock [7,8], a nonplanar dissociation of the dislocation into two Shockley partials and a stair rod dislocation, introduced by Kear and Oblak [9].

The observation of $a\langle 100 \rangle$ dislocations in the γ' -phase of superalloys started with the works of Louchet und Ignat [10] and Bonnet and Ati [11], who investigated CMSX-2 single crystals deformed under $\langle 001 \rangle$ compression. At first sight the results appear very similar to those in single phase material: $a\langle 100 \rangle$ Burgers vectors and $\langle 110 \rangle$ line vectors. The dislocations often show a rectangular bend from one $\langle 110 \rangle$ direction to another. The decisive difference is that $\vec{b}$ is perpendicular to the $\{100\}$ plane, in which the two dislocation segments are lying. This means that the complete dislocation has an edge character, a configuration called prismatic loop. The same result was found in CMSX-4 and CMSX-10 but during creep under $\langle 001 \rangle$ tensile loading [4,12].

Because $\vec{b}$ and the prismatic loop do not have a common plane, the configuration can not glide. Additionally the applied load does not act on these dislocations because the load axis and $\vec{b}$ are perpendicular. This leads to the questions: how are these prismatic loops generated and what role do they play in the creep process? These questions were discussed in detail by Epishin and Link [4]. The explanation of the loop's shape and core structure however is still missing. The B5 lock found in single phase γ' -material and also later in superalloys [13] is restricted to $a\langle 100 \rangle$ dislocations of the 45° type, i.e. it fails to explain for the shape of the $a\langle 100 \rangle$ edge dislocations in superalloys. Jössang *et al.* [14] suggested for fcc crystals a different dissociation in Shockley and stair rod dislocations, now called Hirth lock. A $a\langle 100 \rangle$ edge dislocation dissociates into two $a/2\langle 110 \rangle$ superpartials on two different $\{111\}$ planes which further dissociate into Shockley partials which move away until trapped by the intrinsic stacking fault generated by their movement. The Shockley partials left behind form a $a/3\langle 100 \rangle$ stair rod dislocation in the intersection line of their glide planes. Dislocation loops with $a\langle 100 \rangle$ Burgers vectors and such a core structure were found by Bilde-Sorensen and Leffers [15] in Cu with 10 weight% Ni after radiation damage at 1 MeV and 450 °C. As an explanation for the shape of prismatic loops observed in superalloys the Hirth lock was suggested by Link *et al.* [12], where simple estimations of the dislocation line energies using the theory of elasticity (TE) led to the supposition that this dissociation might be favourable. More precise statements are not possible on this level, because the real structure of the dissociated dislocation is not considered. Molecular dynamics (MD) enables simulation of the dissociation of a dislocation on the atomic level. This method was used to check the strength of Hirth locks in Ni [16], but in our case, due to the $L1_2$ structure of Ni_3Al , the dissociation structures of $a\langle 100 \rangle$ superdislocations should be more complex. Therefore, in the present paper the MD method was applied to the $L1_2$ structure to understand the atomic structure of the $a\langle 100 \rangle$ dislocation core in the γ' -phase. The MD simulations were accompanied by TE calculations in order to extrapolate the MD results up to dimensions which allow us to discuss the relevance of the core structure for the mechanical behaviour. The obtained results fully support the hypothesis that $a\langle 100 \rangle$ edge superdislocations are pinned in $\langle 110 \rangle$ orientation by the Hirth lock.

2. Experimental

[001] single crystals of CMSX-4 and CMSX-10 were creep deformed under uniaxial tensile load. The creep tests were interrupted in different stages and the specimens cooled down under load. Detailed analysis of the dislocation structures in the γ/γ' -interfaces and in the γ' -phase were performed by transmission electron microscopy (TEM) in diffraction contrast. Prismatic loops were found in the γ' -phase after $a\langle 100 \rangle$ dislocations had formed in the γ/γ' -interface in agreement with Eggeler and Dlouhy [3]. A rough identification of the Burgers vectors of the loops was performed by qualitative image analysis of the main and residual

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contrasts. Those dislocations appearing to have $a\langle 100 \rangle$ Burgers vectors were further analysed by image simulation. The investigations are presented in detail by Link *et al.* [12]. The micrographs in Fig. 1 show the characteristic shape of the prismatic dislocation loops in CMSX-4 and CMSX-10 giving rise to the molecular dynamics simulations of the dislocation core structure. Both dislocations have the Burgers vector $a[001]$. Fig. 1a was taken with a $\bar{1}11$ reflection. The dislocation segment appearing as a very sharp line has the line vector $[1\bar{1}0]$ so the residual contrast $\vec{g} \cdot (\vec{b} \times \vec{\xi})$ vanishes. ($\vec{b}$ is Burgers vector, $\vec{\xi}$ is the line vector, $\vec{g}$ is the diffraction vector for the $\bar{1}11$ reflection). The segment with blurred out contrast has the direction $\vec{\xi} = [110]$, so the residual contrast adds to the main contrast $\vec{g} \cdot \vec{b}$. Fig. 1b was taken with a 200 reflection. The $\vec{g}$ -vector forms the same angle with both segments, therefore both show the same contrast. The double line is typical for the residual contrast of $a\langle 100 \rangle$ dislocations under such imaging conditions, as shown by image simulation by Link *et al.* [12] and Dlouhy *et al.* [17].

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Such loops we observed after creep tests longer than about 1/3 of the life time (Fig. 2 and Table 1). Climbing of the loops through the γ' -phase acts as a recovery mechanism making possible further dislocation movement in the matrix channels [4]. The creep curves show that the times after which prismatic loops are observed belong to the creep stages at the onset of accelerated creep until rupture.

3. Molecular dynamics simulations

3.1 Simulation method

The structures and energies of $a\langle 100 \rangle$ edge dislocations in Ni_3Al were found by performing static relaxations of the atoms in MD simulations in order to find the configurations of minimum energy. In classical MD simulations, the atoms are considered as point particles interacting by forces derived from empirical potentials. The trajectories of the atoms in time are obtained by numerical integration of Newton's equations of motion. For intermetallic alloys, Embedded Atom Method (EAM) potentials [19] are an appropriate type of empirical potential. In the present case of Ni_3Al , the potential of Voter and Chen [20] was used. Planar lattice fault energies calculated from this potential are given in Table 2 together with experimental values. While the energy of the (111) antiphase boundary (APB) obtained from the EAM potential is in good agreement with the experimental value, the calculated energy of the complex stacking fault (CSF, $\vec{b} = a/6 \langle 112 \rangle$) is just about half the value of the available experimental result. From this follows that the simulated dissociation widths of dislocations split into partial dislocations involving CSFs can be expected to be twice as large as in real materials. The calculated value of the energy of the superlattice intrinsic stacking fault (SISF, $\vec{b} = a/3 \langle 112 \rangle$), which does not occur in our simulations, is – similar to the experimental value – well below the energy of the APB and CSF.

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Simulations were performed for $a[100]$ edge superdislocations with various line directions. The starting configuration for the simulations is shown schematically in Fig. 3. In a rectangular crystal of Ni_3Al an $a[100]$ edge dislocation along the y axis is generated by removing two (100) lattice half planes. Then a part of the disturbed crystal is deformed in such a way that the gap is closed. The x axis of the simulation box for all simulations corresponds to the $[100]$ direction, but different crystal orientations were used in the (100) plane, i.e. rotations around the $[100]$ axis by the angle θ were performed. For symmetry reasons, only angles θ in the range from 0° to 45° have to be considered such that the y direction varies between the $[010]$ and the $[011]$ direction. In the y direction, the crystal was oriented along $[0kl]$ where

$[0kl]$ is a lattice vector with $k > l$. The corresponding rotation angle is $\theta = \arctan(l/k)$. Along the x and y directions periodic boundary conditions were applied, i.e. effectively the system consists of a row of infinitely long edge dislocation with a distance equal to the extension L_x of the simulation box in x direction. In the z direction, free boundary conditions were used with the constraint that atoms in the lower and upper boundary region can not move in z direction. The box dimensions in x and z directions were chosen to be $L_x = 140a \approx 500$ Å and $L_z \approx 500$ Å, with the lattice parameter a taken as 3.571 Å. In the y direction, the box has the length of the vector $[0kl]$. The total number of atoms N in the simulation box varies between about 340 000 and 1200 000, depending on the values of k and l .

Configurations of minimal energy were obtained in MD simulations using a relaxation algorithm where the atom velocities are set to zero whenever the scalar product of the total velocity and the total force on the atoms in the $3N$ -dimensional configuration space becomes negative, that is, whenever the system moves out of an energy minimum. At the end of a relaxation, the mean force on the atoms was below 10^{-7} eV/Å and the temperature below 10^{-8} K. Besides the atom positions, the total stress tensor of the system was relaxed too by rescaling the simulation box during the simulation in such a way that the total stress tensor of the system attains a prescribed value. In order to find different local energy minima for a dislocation configuration with a given line direction, pre-relaxations with a finite total stress tensor component σ_{zz} in the range from -1 GPa to 1 GPa were performed. The resulting configurations were then relaxed a second time with the constraint of a vanishing stress tensor. Some of the obtained dislocation structures were also relaxed with different values of the total stress tensor in order to investigate the effect of an applied load.

The structures of the resulting dislocations were studied using a Common-Neighbour analysis [23] by which the cores of partial dislocations, CSFs, SISFs, and APBs can be detected. The Burgers vectors of the partial dislocations were determined by computing the relative atom displacements across the glide plane.

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3.2 Results

The structure and energies of the $a[100]$ dislocations were studied for various line directions in the (100) plane. For line directions $\vec{\xi}$ with θ between 0° ($\vec{\xi} = [0\bar{1}0]$) up to about 30° ($\vec{\xi} = [0\bar{5}\bar{3}]$) no clear dissociation of the dislocation core in the relaxed systems can be seen if the total stress has vanished during relaxation. The diameter of the dislocation core is about 10 Å. In the range $\theta > 30^\circ$ up to 45° ($\vec{\xi} = [0\bar{1}\bar{1}]$), three different types of the dissociation of the total dislocation into partials could be discerned as described below. It should be taken into account that for all discussed line directions the dislocation retains its edge character.

We first consider the case of $\theta = 45^\circ$. Two dissociation forms of the $a[100]$ dislocation were found depending on the value of the stress tensor in the pre-relaxation. The configurations are shown in Fig. 4 with the central part of the simulation box projected into the (011) plane. The configuration in Fig. 4a corresponds to the Hirth lock in fcc lattices, reaction number 3 in [14]. A calculation of the displacements of the atoms across the glide planes gives the following dissociation into partials:

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$$a[100] \rightarrow \frac{a}{6}[21\bar{1}] + CSF + \frac{a}{6}[200] + CSF + \frac{a}{6}[2\bar{1}1] \quad (1)$$

The dissociation is shown schematically in Fig. 5a. The width of the dissociation of the two wings of the configuration is about 35 Å, which could be too large by a factor two since the CSF energy following from the EAM potential is too small as described above.

The configuration in Fig. 4b corresponds to a dissociation of the $a[100]$ superdislocation into two $a/2\langle 110 \rangle$ dislocations on two intersecting $\{111\}$ glide planes that enclose the acute angle. The computation of the atom displacements yields the following dissociation:

$$a[100] \rightarrow \frac{a}{6}[112] + CSF + \frac{a}{6}[2\bar{1}1] + APB + \frac{a}{6}[21\bar{1}] + CSF + \frac{a}{6}[1\bar{1}2] \quad (2)$$

presented in Fig. 5b. The APB is not visible in Fig. 4b. This configuration is called type II in the following text, the dissociation in Fig. 4a is called type I. Type II corresponds to a dissociation forming a wedge that opens up in the positive $[100]$ direction. A wedge opening up in the negative $[100]$ direction is equivalent. Which one of these configurations forms in the simulation depends on the starting configuration. This does not prove right for type I, where a wedge open in $[01\bar{1}]$ direction needs to have a Burgers vector with opposite sign. While the dissociation of type I yields a configuration that is stable in the fcc structure too (Hirth lock), the configuration of type II exists exclusively in the $L1_2$ structure. The superlattice is the prerequisite for the formation of the APB, which prevents the gliding of the $a/2\langle 110 \rangle$ dislocations, thus stabilising this configuration.

For dislocation line directions forming an angle θ of about 30° up to 45° with the $[0\bar{1}0]$ direction, two configurations have been found being similar to type I and II (Figs 6a, b). The dissociation into partial dislocations proceeds not just on one $\{111\}$ glide planes but one neighbouring $\{111\}$ planes. The $a/3\langle 111 \rangle$ jump from one plane to the next, called a jog, presents an extended additional lattice imperfection. Figs 6a, b show these dislocations in the case of the line direction $[0,10,9]$ corresponding to $\theta \approx 42^\circ$. The length of the part of the dislocation line residing on a single glide plane, that is, the period p of the configuration is given by

$$p = \frac{a}{\sqrt{2} \sin(45^\circ - \theta)} \quad (3)$$

since the distance between two adjacent (111) planes, measured in the direction perpendicular to $[011]$ in the plane formed by $[011]$ and $[0k\bar{l}]$, is $a/\sqrt{2}$.

A third configuration has been found that shall be designated as type III and is shown in Fig. 6c. It corresponds to two $a/2\langle 110 \rangle$ dislocations that are interlocked with a period p given by Eq. (3). The configuration of type III does not exist for $\theta = 45^\circ$ since its period in this case is infinite preventing an interlocking. Similar to the structure of type II, the dissociation of type III is not expected to exist in the fcc structure.

The energy of a dislocation can only be defined if an outer cutoff radius is specified since the strain field of a dislocation is long range and the energy stored in the strain field within a cylinder of radius R around the dislocation line diverges logarithmically with R . The dislocation line energy $W(R)/L$ per unit length is here defined as the potential energy of the atoms within the cylinder minus the cohesive energy of these atoms. Thus,

$$\frac{W(R)}{L} = \frac{E_{pot}(R) - N_{Ni}E_{Ni}^0 - N_{Al}E_{Al}^0}{L} \quad (4)$$

where $E_{pot}(R)$ is the sum of the potential energies of all atoms contained in a cylinder of radius R with the dislocation in the center. N_{Ni} and N_{Al} are the numbers of Ni and Al atoms contained in the cylinder and $E_{Ni}^0 = 4.485$ eV and $E_{Al}^0 = 4.782$ eV are the cohesive energies of Ni and Al in the $L1_2$ structure given by the EAM potential. L is the length of the dislocation line in the simulation box. In Fig. 7, the line energy $W(R)/L$ is plotted for four different dislocation line directions where for $\theta > 30^\circ$ the type I dislocation structures were used¹.

¹ For the dissociated dislocation the center of the stair rod dislocation is chosen as the origin, $R=0$.

It can be seen that the shape of the energy curves for $R < 50 \text{ \AA}$ depends on the line direction while for larger cutoff radii the energy curves seem merely to be shifted against each other. This means that the energy differences of the dislocations are mainly determined by the dissociation geometry of the dislocation, which is different for the four cases shown in Fig. 7. The line energy $W(R)/L$ then consists of two parts, the energy of the dissociation and the contribution of the long range strain field where the latter part is only weakly depending on the line direction. In order to compare the dependency of the dislocation energies on the line direction for different dissociation types we chose R to be $100 \text{ \AA}$ and took the energy of the dislocation of least energy as the reference point for the dislocation energies. This turned out to be type I with $\theta = 45^\circ$, i.e. the Hirth lock. The energy differences $\Delta W/L$ between the energies of the other dissociation types X , $W/L(\theta, \text{type} X)$, and the reference point $W/L(45^\circ, \text{type I})$ was calculated as a function of the line direction (Fig. 8). It can be seen that the dislocation energies are generally decreasing with increasing orientation angle θ . For $\theta = 45^\circ$ corresponding to the line direction $[0\bar{1}\bar{1}]$, there is a clear minimum of the energy. Dislocations dissociated according to type I have the minimum energy of all types of dissociation for a given angle. The energy of dislocations dissociated according to type II have a higher energy with the energy difference increasing with θ . Dissociation type III corresponds to the state of highest energy but the energy difference with respect to the type II dislocation is small.

The results of simulations of the dissociation structures of type I and type II with line direction $[0\bar{1}\bar{1}]$ for several applied loadings will be discussed in section 5.

4. Theory of elasticity calculations

The motivation for using MD simulations was to attain information about the dissociation of $a < 100 \rangle$ dislocations. Another important information however is the total energy of the dislocation, depending on the radius R of a cylinder around the dislocation, used as the integration volume. Here the MD simulations reach their limits, because the simulation boxes are small ($R \sim 250 \text{ \AA}$) compared to a quarter of the thickness of the γ' -rafts, about $1250 \text{ \AA}$, being a measure for the outer cutoff radius for the γ' -dislocation in superalloys². Therefore MD simulations were accompanied by TE calculations in order to extrapolate the MD results for higher scales.

First the energy curves determined by MD simulations were compared with the logarithmic law following from analysis of the elastic strains in an infinite continuum containing a single Volterra dislocation [24]:

$$\frac{W(R)}{L} = \frac{Kb^2}{4\pi} \ln \frac{\alpha R}{b} \quad (5)$$

where K is an energetic factor determined by the elastic properties of the continuum and α is a parameter that takes the core energy into account. Dislocation core means the central strongly distorted area of a dislocation with a radius of $\sim |\bar{b}|$, where linear TE can not be applied. The area including the stair rod dislocation and the Shockley partials we call dissociation area. K depends on $\bar{\xi}$ due to the elastic anisotropy of Ni_3Al but in the considered case ($\bar{b} = a[100]$ and $\bar{\xi} = [0kl]$) this dependence is not strong: K monotonically increases by about 6.4% with a change of θ from 0° up to 45° .

In Fig. 9 the MD energetic curves for the dislocations with line vectors $[00\bar{1}]$ and $[0\bar{1}\bar{1}]$ are shown in semilogarithmic coordinates. It is seen that for every MD curve there is an inter-

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² The γ/γ' -interfaces are densely covered with dislocations while the γ' -phase is nearly dislocation free. So the nearest neighbour of a γ' -dislocation is an interfacial dislocation.

val $R_{min} \leq R \leq R_{max}$, where it is nearly straight, which means that it obeys the logarithmic dependence. Beyond these intervals the MD curves are nonlinear, at $R < R_{min}$ obviously due to the dissociation ("dissociation effect") and at $R > R_{max}$ presumably due to the applied boundary conditions ("boundary effect"). The straight lines in Fig. 9 show the logarithmic law (5). The factor $Kb^2/4\pi$, which determines the slope, is equal to the calculated theoretical value, 0.714 eV/Å for $\vec{\xi} = [00\bar{1}]$ and 0.760 eV/Å for $\vec{\xi} = [0\bar{1}\bar{1}]^3$. The parameter α , responsible for a vertical shift, was fitted. For the $[00\bar{1}]$ orientated dislocation the MD curve exactly coincides with the logarithmic law (5) with $\alpha=0.34$ within the linearity interval $4 \text{ Å} \leq R \leq 100 \text{ Å}$. Thus calibrating Eq. (5) by the MD results (determining α), one can extrapolate this energetic curve for large values of R , which is relevant for the real structure. For the $[0\bar{1}\bar{1}]$ orientated dislocation, even within the linearity interval $40 \text{ Å} \leq R \leq 100 \text{ Å}$, the slope of the MD curve is about 20% larger than it is for the Volterra dislocation. Thus, in this case the overlap of the core and boundary effects makes it impossible to perform a reliable calibration of Eq. 5.

To solve this problem, the continuum model was refined to take into account the dissociation effect. The core of each partial dislocation was taken as a cylinder with a radius equal to its Burgers vector, the core energy W_{core}/L was assumed to be equal to $(Kb^2/4\pi) \cdot \ln \alpha$ and uniformly distributed within the core with the density:

$$\rho_{core} = (K/4\pi^2) \cdot \ln \alpha \quad (6)$$

Outside the core the CSF energy and the elastic energy contribute to the total line energy. Fig. 10 shows the configuration of the modified continuum model used for analysis of the Hirth lock. Here the total energy $W(R)/L$ of a cylinder of radius R consists of the energies of the areas $S_n(R)$ of the cores (n is the core number) belonging to the cylinder as well as the CSF energies and the energy of the total elastic strain field $\varepsilon_{ij}(\vec{r})$ resulting from all dislocations:

$$\frac{W(R)}{L} = \sum_n \int_{S_n(R)} \rho_{n-core} d\vec{r} + 2\gamma_{CSF} w_{CSF}(R) + \int_{S(R)} \frac{1}{2} c_{ijkl} \varepsilon_{ij}(\vec{r}) \varepsilon_{kl}(\vec{r}) d\vec{r} \quad (7)$$

Where γ_{CSF} is the specific surface energy of the CSF, $w_{CSF}(R)$ is the CSF width within the cylinder of radius R , c_{ijkl} are elastic constants and $S(R)$ is the area of the cylinder cross-section except the cores. The stress fields of the dislocations were calculated using formulas derived by Spence [25]. Eq. 7 was also used for the undissociated $[00\bar{1}]$ orientated dislocation but without the second term.

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Fig. 11 shows the results for the same dislocations as in Fig. 9. The refined continuum model describes well the core effect and hereby can be calibrated also for the $[0\bar{1}\bar{1}]$ orientation. The fitted values of α are 1.9 for the stair rod dislocation and 1.1 for the Shockley partials. The distance between the stair rod dislocation and the Shockley partials was also adjustable and found to be equal to 30 Å. Calculations for large values of R show that the energetic curve for the $[0\bar{1}\bar{1}]$ orientated dislocation asymptotically converges to the logarithmic law (5) with $\alpha \approx 1.2$ and crosses the $[00\bar{1}]$ energetic curve at R of about few mm, which means that for real dislocation densities $W_{[0\bar{1}\bar{1}]} / L$ is always smaller than $W_{[00\bar{1}]} / L$. The change of the energy ratio $W_{[0\bar{1}\bar{1}]} / W_{[00\bar{1}]}$ with R is shown in Fig. 12. This ratio is small at R close to the radius of the dislocation area but rapidly increases with increasing R reaching nearly a plateau with a level of about 0.9 at $R=1000 \text{ Å}$, which can be used as a reasonable estimation of $W_{[0\bar{1}\bar{1}]} / W_{[00\bar{1}]}$ for superalloys.

³ The lattice spacing and the elastic constants are equal to those following from the MD simulations.

It should be mentioned that in reality the core shape is not circular. E.g. it follows from the MD simulations that the cores of partials are stretched along the glide plane as it is in the Peierls-Nabarro model [26]. But in spite of this idealisation the applied continuum model gives reliable results from the energetic curves, obviously due to the integration effect.

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5. Discussion

It follows from the performed MD simulations that the $a\langle 100 \rangle$ edge dislocations attain in the γ' -phase the preferential $\langle 110 \rangle$ orientation because in this orientation they dissociate and thereby attain the minimum line energy. The dissociation of the perfect dislocation into partials results in a strong decrease of the core energy, which is the main contribution to the energy gain. In terms of the continuum modelling it can be interpreted as a decrease of the density of the core energy (see Eq. (6), α decreases from 3.4 for the undissociated $[00\bar{1}]$ orientated dislocation down to 1.9 and 1.1 for the stair rod dislocations and Shockley partials respectively) as well as a reduction of the total area of the dislocation cores ($\sum_n \pi b_n^2 : \pi \left(\sum_n b_n \right)^2 = 4/9$). The dissociation also decreases the elastic energy by splitting a peak of the elastic strains at the dislocation core ($\left(\sum_n \varepsilon_n \right)^2 > \sum_n \varepsilon_n^2$ effect). However this effect is relevant only inside and in the vicinity of the dissociation area.

At the distances larger than $R \approx 100 \text{ \AA}$ the change of the local elastic energy due to the dissociation is insignificant. Here the higher density of the elastic energy W_{el} for the $[0\bar{1}\bar{1}]$ orientation compared with the $[00\bar{1}]$ orientation becomes important. It follows from (5) that with increasing radius R the elastic energy W_{el} of the dislocation with $[0\bar{1}\bar{1}]$ line vector grows faster than that with $[00\bar{1}]$ line vector: $dW_{el}/dR \sim K$, $K_{[0\bar{1}\bar{1}]} > K_{[00\bar{1}]}$. Therefore with an increase of R the energy gain of the $[0\bar{1}\bar{1}]$ orientated dislocation decreases (Fig. 12).

Based on the obtained estimation of the line energy of the $a[100]$ dislocation, the formation mechanism of prismatic loops in the γ' -phase can be discussed. It was shown in [4] that $a[100]$ dislocation segments first form in the γ/γ' -interface and then bow and enter the γ' -phase as prismatic loops. When the $[001]$ orientated interfacial segment with length l form the $\langle 011 \rangle$ shaped loop of the length $\sqrt{2}l$ the energy increases by $(\sqrt{2} - 1.1) \cdot W_{[011]}/L$ (1.1 is the energy ratio $W_{[001]}/W_{[011]}$). During creep of superalloys with rafted γ/γ' -microstructure the harder γ' -phase constrains the softer γ -phase which results in transverse stresses. Under tensile load ($\sigma_a > 0$) the transverse stress $\sigma_{\perp}$ in the γ' -phase becomes rapidly compressive and after primary creep remains nearly constant reaching a value close to $-\sigma_a$ [27,28]. During the formation of a prismatic loop this stress produces a mechanical work equal to $-\sigma_{\perp} \cdot a \cdot A$, where $A = l^2/4$ is the loop area. This allows us to calculate the critical segment length l_{cr} , below which the mechanical energy is not sufficient for generating the prismatic loop:

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$$l_{cr} = - \frac{4(\sqrt{2} - 1.1) W_{[011]}}{a \cdot \sigma_{\perp} L} \quad (8)$$

For $l > l_{cr}$ the interfacial network loses its stability and the $a\langle 100 \rangle$ dislocations enter the γ' -phase.

Taking $\sigma_{\perp} \approx -\sigma_a = -120$ MPa and $W_{[011]}/L = 4$ eV/Å = $6.4 \cdot 10^{-9}$ J/m one gets $l_{cr} \approx 1800$ Å. This value is several times larger than that ($l \approx 500$ Å) for which the γ' -entering process is observed under this applied stress [12]. Thus, $\sigma_{\perp}$ is not strong enough to push an $a[100]$ interfacial segment into the γ' -phase and it has to be supported by the osmotic force of vacancies generated in the γ/γ' -interface as proposed by Epishin and Link [4] or by repulsive forces of neighbouring dislocations.

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The presented calculations were performed for load free condition. For the deformation behaviour, however, it is important how stable the Hirth lock is under applied load. Baskes *et al.* [16] showed that under load the Hirth lock in Ni changes its configuration and can even collapse. In the γ' -phase of creep deforming superalloys the stress state is different from that considered by these authors, therefore the stability of the Hirth lock during creep was investigated. From TE it follows that the distance w between the stair rod dislocation and the Shockley partials is determined by

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$$w = \frac{G}{\gamma_{CSF} - F_{gl}/L} \quad (9)$$

The parameter G depends on the elastic constants and describes the repulsive forces between the dislocations. F_{gl}/L is the glide component of the elastic force acting on the Shockley partials due to the stress σ . For superalloy single-crystals creep deforming under uniaxial stress σ_a applied in $[001]$ direction the stress tensor σ in the γ' -phase is:

$$\sigma = \begin{pmatrix} \sigma_{\perp} & 0 & 0 \\ 0 & \sigma_{\perp} & 0 \\ 0 & 0 & \sigma_a \end{pmatrix} \quad (10)$$

which causes the glide force on the Shockley partials:

$$\frac{F_{gl}}{L} = \frac{a}{6\sqrt{3}}(\sigma_a - \sigma_{\perp}) \approx \frac{a}{3\sqrt{3}}\sigma_a \text{ for } \sigma_{\perp} \approx -\sigma_a \quad (11)$$

Therefore under such a stress tensor the dissociation width w of the Hirth lock increases as presented in Fig. 13. The TE results were compared with MD calculations. Fig. 13 shows that both give similar dependencies of $w = f(\sigma_a)$ but the obtained values of the parameter G are somewhat different: $G=40.1$ GN for MD and $G=32.9$ GN for TE. The reason could be that Burgers vectors are distributed within the dislocation cores (like in the Peierls-Nabarro model), while in the Volterra dislocation it is assumed to be point distributed in the dislocation center. This difference should be taken into account during experimental measurement of γ_{CSF} , when the TE formula (9) is used, especially when w is comparable with the core size of the Shockley partials and a stair rod dislocation. When F_{gl}/L reaches γ_{CSF} the partials are no longer locked by the stair rod dislocation and the Hirth lock disintegrates. According to (9) this is the case for stresses of about 2000 MPa, which is however beyond the ultimate tensile stress of superalloys and therefore never occurs. For realistic stress levels (<200 MPa), as usually applied during creep tests at temperatures $\geq 1000^\circ\text{C}$, the relative increase of the dissociation width $\Delta w/w$ does not exceed 12%.

It follows from the above results that the formation of the Hirth lock is the reason for the $\langle 011 \rangle$ line direction of $a[100]$ prismatic loops in the γ' -phase and that this configuration remains stable during creep. The relevance of such a lock of course depends on how much it blocks the movement of the dissociated dislocation. Such a blocking however assumes, that the dislocation propagates by glide, not by climb as in the considered case. Therefore the influence of the core structure on diffusion controlled climb has to be discussed.

It is usually assumed that climb is controlled by lattice diffusion but in case of lower temperature it is also assumed that climb could be controlled by the core diffusion when the lat-

tice diffusion is slow (e.g. [29]). Huang *et al.* [30] showed by MD that the core diffusion in Cu is slower in dissociated dislocations. For the lattice diffusion the wide dissociated core can work as an effective trap of the lattice vacancies. In this case the CSF wings receive a wide flux of vacancies, which then rapidly move along the CSF to the dislocations. So if core diffusion dominates the Hirth lock slows down the climb rate, but if lattice diffusion is stronger it has the opposite effect. It is known that the lattice diffusion in an ordered structure like Ni₃Al is slow (e.g. [31]) but on the other hand 1100°C is a very high temperature (for CMSX-4 it corresponds to the homologous temperature 0.82) where the climb in the γ' -phase should be controlled by lattice diffusion. Thus in the considered case the Hirth lock is expected to accelerate the climb of the $a\langle 100 \rangle$ dislocation through the γ' -raft.

The three-dimensional image of the Hirth lock in Fig. 6 shows jogs. Jogs play an important role in climb processes by reducing the energy required for the dislocation movement. According to Eq. (3) the period of the jogs increases when the line direction approximates $\langle 011 \rangle$. Thus these jogs should play a role during the transition from the interfacial dislocation into the prismatic loop, but when the $\langle 011 \rangle$ line direction is attained they should disappear.

The found dissociation of type II (Figs 4b, 5b and 6b) has a similar configuration as the dissociation of a $a[010]$ edge dislocation proposed in the publication of Srinivasan *et al.* [18]. The authors applied high resolution TEM, using phase contrast, to visualize the core structure of an $a[010]$ dislocation with $[10\bar{1}]$ line vector formed under $\langle 110 \rangle \{111\}$ shear loading. The TEM image of the core is interpreted as dissociation of an $a[010]$ dislocation into $a/2[011]$ and $a/2[0\bar{1}\bar{1}]$ partials, gliding on two different $\{111\}$ planes. The glide planes form an acute angle like in our dissociation of type II, the $a/2 \langle 011 \rangle$ partials, however, are not additionally dissociated into Shockley partials. They do not form stacking faults but they are connected by an APB with a width of about 25 Å. So in our type II dissociation and that of Srinivasan *et al.* [18] an APB, not a stair rod dislocation like in the Hirth lock, locks the dislocations, which are dissociated on two different $\{111\}$ planes, forming an acute angle. In our case the $a/2 \langle 110 \rangle$ dislocations are widely dissociated into Shockley partials and the APB is small, in their case opposite. The glide movement of the $a/2 \langle 011 \rangle$ dislocations is restricted by the high energy APB. In their model further movement is expected to take place by climbing back to the (101) plane, which is in-between the (111) and $(\bar{1}\bar{1}1)$ glide planes (i.e. it forms an angle of 35° with both $\{111\}$ planes.) This zigzag movement of the $a \langle 011 \rangle$ dislocations has in total the effect that the $a \langle 001 \rangle$ dislocation moves on a $\{110\}$ plane. The reason for the observed splitting is according to Srinivasan *et al.* [18], that by $\langle 110 \rangle \{111\}$ shear loading one specific octahedral glide system is activated. Indeed the observed splitting showed that one of the two $a/2 \langle 011 \rangle$ dislocations has such a Burgers vector and glide plane. Their explanation for the $\langle 110 \rangle$ line direction uses geometrical considerations. The coupled glide/climb process makes necessary two different $\{111\}$ planes, intersecting with such a line direction.

The dissociation of type II was found to have a higher energy than the dissociation of type I (Fig. 8), and, therefore, one should expect that the formation of the Hirth lock is preferable under load free condition. The energies of these dissociations are, however, influenced by applied load. MD calculations showed that under loading given by the stress tensor (10) the dissociation of type II becomes unstable and transforms into the Hirth lock, when the applied stress σ_a reaches 450 MPa. Thus it is possible that depending on the loading conditions, the $a \langle 001 \rangle$ dislocation dissociates by type I or II. The compressive transverse stresses induced in the γ' -phase during uniaxial tensile creep result in the dissociation of type I, while creep under $\langle 110 \rangle \{111\}$ shear loading probably leads to the dissociation of type II.

The TEM micrographs, presented in Fig. 1 are taken in bright field diffraction contrast. They show unequivocally the $\langle 011 \rangle$ line direction, the $a \langle 100 \rangle$ Burgers vector and the edge character of the γ' -dislocations. The resolution however is not sufficient to provide informa-

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tion about the core splitting. For that purpose further high resolution TEM investigations are planned.

6. Conclusions

It was found by energy minimization in MD simulations that $a[100]$ edge superdislocations lying in the (010) plane of Ni_3Al dissociate when the line direction approaches the [011] orientation. Three types of dissociation are found: a symmetric dissociation similar to the Hirth lock in fcc structures, an asymmetric dissociation, and a dissociation into two interlocked $a/2\langle 110 \rangle$ dislocations. The Hirth lock is the lowest energy configuration.

The reasons for the dissociation are a strong energy reduction due to the core splitting and relaxation of elastic strains within the dissociation area.

From TE calculations it follows that the total energy gain due to the change of the dislocation orientation from [001] to [011] and the dissociation into the Hirth lock decreases when the cutoff radius R increases, but it remains positive for interdislocation distances typical for deformed superalloys.

MD and TE simulations show that under loading conditions typical for creep tests of nickel-base superalloys at high temperatures ($\geq 1000^\circ\text{C}$), the Hirth lock somewhat expands but remains stable. The asymmetric configuration is less stable and even transforms into the Hirth lock under certain loading conditions.

The combination of MD simulations and TE calculations allows us to extrapolate the MD results for longer dislocation distances, typical for real structures, and gives a physical understanding of the results obtained by simulation.

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Superalloy	Temp. [°C]	Load [MPa]	Norm. time	Strain [%]	Creep stage	Testing type	Reference
CMSX-10	1100	$\sigma=120$	0.36	1.6	transition steady $\rightarrow$ accelerated creep	[001]-creep, tension	This paper
CMSX-4	1050	$\sigma=180$	0.80	7.1	accelerated creep		
	1100	$\sigma=120$	0.38	1.3	middle of steady creep		
CMSX-4	1020	$\tau=80$		15		Shear creep, <011>{111}	[18]
CMSX-2	975	$\sigma=200$ - 400		4		[001]-creep, compression	[10]
CMSX-2	900			1		Dynamical compression	[11]
CMSX-6	1025	$\tau=85$		20		Shear creep, <011>{111}	[3]

Table1. Creep test parameters of CMSX-superalloys, where prismatic loops were observed. The testing time is normalised by the rupture time to allow comparison between different tests. For the tension and compression test the stress σ is given, for shear tests the shear stress τ .

Lattice fault	EAM	Experimental, reference	
(111) APB	157	180	[21]
CSF	134	250	[22]
SISF	43	5-15	[21]

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Table 2. Planar lattice fault energies in mJ/m^2 for the (111) antiphase boundary (APB), the complex stacking fault (CSF), and the superlattice intrinsic stacking fault (SISF) in Ni_3Al obtained from calculation using the EAM potential and from experiments.

Figure captions

Figure 1: $a\langle 100 \rangle$ prismatic loops in the γ' -phase during high temperature creep. Left: CMSX-10, 1100°C, 120 MPa, 200 h. Beam direction $\vec{k}_0 = [1\bar{1}2]$, $\vec{g} = (\bar{1}11)$. Right: CMSX-4, 1100°C, 120 MPa, 150 h. $\vec{k}_0 = [001]$, $\vec{g} = (200)$.

Figure 2: High temperature creep curves of CMSX-4 and CMSX-10. Conditions where $a\langle 100 \rangle$ dislocations were observed are marked by arrows.

Figure 3: Scheme of the simulation box. The shaded regions indicate atoms which are restricted to move in the x - y plane.

Figure 4: Projections onto the (011) plane for an obtuse (a) and an acute (b) dissociation of $a[100]$ dislocations. The line direction $[0\bar{1}\bar{1}]$ is perpendicular to the projection plane, i.e. the dislocation is in edge on position. Black atoms are in the cores of partial dislocations, grey atoms in stacking faults, and white atoms in the defect free region. The atoms are coloured regardless of the atom types.

Figure 5: Schematic drawing of the dissociations of an $a[100]$ dislocation with line direction $[0\bar{1}\bar{1}]$ into partial dislocations. Complex stacking faults are indicated by dashed lines.

Figure 6: Three different dissociations of $a[100]$ dislocations with line direction $[0\bar{1}0, \bar{9}]$. Light atoms denote atoms in the stacking faults and dark atoms mean atoms in the cores of partial dislocations. The period of the configurations is $p = 48 \text{ \AA}$. The length of the dislocation segments shown is $192 \text{ \AA}$.

Figure 7: Line energies as a function of the cutoff radius R of $a[100]$ dislocations with four different orientations of the dislocation lines.

Figure 8: Relative energies $\Delta W(R)/L$ of $a[100]$ dislocations for different line directions given by the angle α and for different dissociation types. The energies correspond to the cut-off radius $R = 100 \text{ \AA}$ and the energy of the Hirth lock (indicated by an arrow) is taken as the reference energy.

Figure 9: Comparison of the MD energetic curves with the logarithmic law for dislocations with line vectors $[00\bar{1}]$ and $[0\bar{1}\bar{1}]$.

Figure 10: Refined continuum model for a dissociated $a[100]$ dislocation with line direction $[0\bar{1}\bar{1}]$.

Figure 11: The energetic curves for the $[00\bar{1}]$ and $[0\bar{1}\bar{1}]$ orientated dislocations calculated by molecular dynamics (MD) and by the refined continuum model.

Figure 12: Ratio of the line energies for $[0\bar{1}\bar{1}]$ and $[00\bar{1}]$ orientated dislocations as a function of the radius R of the surrounding cylinder.

Figure 13: Expansion of the Hirth lock in superalloy single-crystals loaded in $[001]$ direction

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228x169mm (72 x 72 DPI)

270x146mm (72 x 72 DPI)

313x127mm (72 x 72 DPI)

300x123mm (72 x 72 DPI)

292x147mm (72 x 72 DPI)

Review Only

10x7mm (600 x 600 DPI)

10x7mm (600 x 600 DPI)

Peer Review Only

224x165mm (72 x 72 DPI)

218x157mm (72 x 72 DPI)

223x164mm (72 x 72 DPI)

231x165mm (72 x 72 DPI)

226x167mm (72 x 72 DPI)