Criticality in the Plastic Deformation of Ni_3Al

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It is argued that the critical point of a nonequilibrium phase transition in the motion of dislocations results in the experimentally observed power-law creep rates in Ni_3Al and related intermetallic alloys. A simple scaling argument is used to connect the critical exponents of the transition directly to the creep rate. A model of dislocation motion is constructed. The exponents predicted from the model are in agreement with those deduced from creep experiments.

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The study of nonequilibrium phase transitions has become an important part of modern physics [1]. It is argued below that the superdislocations (henceforth referred to as "dislocations") responsible for the plastic deformation in Ni_3Al and related intermetallic alloys undergo a nonequilibrium phase transition. A scaling argument is used to connect the critical exponents of the transition to the mechanical properties of the alloy. A simple creep experiment, in which the strain is measured as a function of time for a sample subject to a constant stress, directly measures one of the critical exponents of the transition. A model of dislocation motion is constructed and yields exponents that are in excellent agreement with experimentally measured values.

Ni_3Al is the prototype of a class of technologically important $L1_2$ intermetallic alloys which differ from pure metals in that their plastic strength increases with temperature [2]. (The following arguments apply to all alloys in this class, but for brevity only Ni_3Al is explicitly mentioned.) The movement of dislocations is the primary microscopic mechanism of plastic deformation in single crystals [3]. The observed plastic strength increase in Ni_3Al has been linked to the thermally activated formation of cross-slip points—segments of dislocations which cross slip from easy glide {111} planes onto {001} planes where they are immobilized—along the dislocations [4]. As the temperature increases, cross-slip pinning becomes more frequent, impeding the motion of the dislocations.

Paidar, Pope, and Vitek [5] have analyzed the formation of an isolated pinning point. It was found that, in order to cross slip, a dislocation must have sufficient screw character. Also, as a dislocation bows about a pinning point, it exerts a force on the pinning point. Eventually, this force reaches a critical value, at which the pinning point dissolves. The energy stored in a bowing dislocation creates a stress opposing the applied stress. If two pinning points form near each other, the bowing stress prevents dissolution of either pinning point, and the segment of dislocation between the points becomes immobile.

Recently, the formation of pinning points has been incorporated into a simulation of dislocation motion that accurately reproduces the experimentally observed microstructure [6]. More importantly, the simulations allow the study of the dynamics of dislocation motion. At low stresses, the dislocations advance in the screw direction through the lateral motion of mostly edge-character segments referred to as superkinks [labeled as "SK" in Fig. 1(a)], while the remaining, highly pinned segments remain stationary. Ultimately, the highly pinned segments encompass the entire dislocation and immobilize it. This exhaustion of mobile dislocations is proposed as the origin of work hardening in Ni_3Al. At higher stresses, the advancement of dislocations occurs more uniformly by forward bowing between pinning points [Fig. 1(b)], as envisioned in prior modeling efforts [5]. In this stress regime, a mobile dislocation remains mobile for an extended time. The difference in the mode of dislocation motion is related to the stress dependence of the correlations between pinning events. Figure 1(c) depicts the origin of

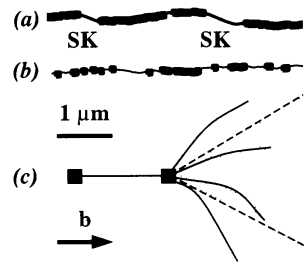

FIG. 1. (a),(b) Simulated dislocation configurations of near screw character (the Burgers vector **b** is indicated) typical of those found below and above the critical stress, respectively. Below the critical stress, the pinning (represented by solid points) along the dislocation is highly correlated and the dislocation advances through the lateral motion of the unpinned segments referred to as superkinks (SK). In this case, the superkinks move to the right. Above the critical stress the pinning is less correlated and the dislocation moves more uniformly, through the forward bowing of the unpinned segments. (c) The origin of the correlations. Near any given pinning point there is only a small region (shaded) of space within which a pinning point can form and exhaust a dislocation segment. The presence of a pinning point forces the dislocation to bow, reducing its velocity. The reduced velocity increases the time spent in the pinning region and enhances the probability of pinning.

these correlations. A dislocation segment can be immobilized if a new pinning point forms near a preexisting one. Since cross slip can only occur near screw orientation, the new pinning point must form within the shaded region. At low stresses, the moving segment adjacent to a pinning point spends disproportionately more time in the pinning region than an equivalent segment at higher stresses, enhancing the correlation between pinning events [6]. Above a critical stress it is no longer possible for the correlations to create the highly pinned structure of Fig. 1(a). The changes in both dislocation structure and mode of advancement occur rapidly with increasing stress, suggesting a nonequilibrium phase transition.

A simplified argument yields insight into the origin of this transition. In general, plastic strain is proportional to the area swept out by the dislocations. To a rough approximation, the creep rate (i.e., the time derivative of the strain measured in a creep experiment) in the low-stress regime is proportional to the number of mobile superkinks. Let the number of mobile superkinks at time t be denoted by $N(t)$. Earlier modeling efforts [6] suggest three processes that can change the number of mobile superkinks: (i) a mobile superkink spawns an additional mobile superkink, (ii) a mobile superkink becomes immobile, and (iii) a superkink-superkink scattering event reduces the number of mobile superkinks. The rates of processes (i) and (ii) are independent of the number of superkinks. The rate of process (iii) is proportional to the number of superkinks (the rate of superkink-superkink collisions scales inversely as the average superkink separation). The equation describing the time dependence of the average number of mobile superkinks is

$$\dot{N}(t)=[\mu-\omega N(t)]N(t)\,, \tag{1}$$

where the first term in brackets on the right is the net rate of processes (i) and (ii), and the second term is the rate of process (iii). Superkink-superkink collisions can never increase the number of superkinks; ω is always positive. Processes (i) and (ii) combined can either produce a net decrease or increase in the number of mobile superkinks (depending on the applied stress), so μ can have either sign. If $\mu>0$, the steady-state creep rate becomes proportional to μ/ω [7]. If $\mu<0$, the number of mobile superkinks approaches zero, as does the creep rate. The stress at which $\mu=0$ is the critical stress for this nonequilibrium phase transition. At the critical stress, the number of mobile superkinks as a function of time becomes

$$N(t)=(1/N_0+\omega t)^{-1}\,, \tag{2}$$

where N_0 is the initial number of superkinks. In the limit that N_0 becomes infinite, the creep rate becomes proportional to t^{-1}.

The above heuristic argument establishes several salient features of the proposed nonequilibrium phase transition. Below the critical stress, the steady-state creep rate is zero and above the critical stress, a nonzero constant. At the critical stress, the creep rate displays a power-law dependence on the time (deemed a "power-law creep rate," not to be confused with "power-law creep" which is used to characterize the stress dependence of the creep rate). If one considers $N(t)$ to describe the number of mobile dislocations instead of superkinks, this argument suggests that criticality may also be the source of the ubiquitous power-law creep rates in pure metals [8]. A more precise argument for Ni_3Al is presented in the following.

In Ni_3Al, the quantity controlling the creep rate is the number of mobile dislocations. As stated above, for stresses below the critical stress, all dislocations eventually become immobile. Consider a crystal with a large number of dislocations. Imagine the crystal is prestrained in the low-stress regime until it no longer creeps. The stress is then incremented and held fixed. As a result of the increase in stress, immobile dislocations are now mobile, move by the lateral motion of superkinks, and eventually become immobile. Let $n(a,t)da\,dt$ be the number of dislocations which sweep out an area between a and $a+da$ before arresting at a time between t and $t+dt$. Since the strain is proportional to the total area swept out by all of the superdislocations, the creep rate $\dot{\gamma}(t)$ is proportional to

$$\dot{\gamma}(t)\sim\frac{dA(t)}{dt}=\int_t^\infty\frac{dt'}{t'}\int_0^\infty da\,a\,n(a,t')\,, \tag{3}$$

where $A(t)$ is the total area swept out by all of the superdislocations at time t.

It is postulated that, at the critical point, the distribution of event sizes is scale invariant:

$$\lambda n(a,t)=n(\lambda^{\alpha}a,\lambda^{\delta}t)\,, \tag{4}$$

where α and δ are the scaling exponents. Multiplication of both sides of Eq. (3) by λ and using the identity in Eq. (4), one can show that at the critical point $\dot{\gamma}(t)$ is scale invariant:

$$\Lambda\dot{\gamma}(t)=\dot{\gamma}(\Lambda^{\delta/(1+2\alpha)}t)\,, \tag{5}$$

where $\Lambda=\lambda^{1+2\alpha}$. Choosing $\Lambda^{\delta/(1+2\alpha)}=t^{-1}$ in Eq. (5) shows that, at the critical point, the creep rate has a simple power-law dependence on time:

$$\dot{\gamma}(t)\sim t^{-\Delta},\ \text{with}\ \Delta=-(1+2\alpha)/\delta\,. \tag{6}$$

The experiments of Thornton, Davies, and Johnston, performed in 1970, directly measured power-law creep rates. Determining the scaling exponents of the transition is equivalent to *predicting* the algebraic form of the creep curve. Furthermore, a power-law creep rate is the signature of the scale invariance of the distribution of exhaustion events *independent of the underlying exhaustion mechanism.*

A remarkable feature of critical exponents is that they do not depend on the precise microscopic nature of the in-

teractions, but instead are determined by general symmetries. In order to determine the exponents of the proposed nonequilibrium phase transition in Ni_3Al, the following simple model of dislocation motion was developed to approximate the superkink processes (i)-(iii) described above. The dislocation is assumed to consist of L segments, labeled by the index i. Each segment i rests at a position y_i, restricted to be an integer. At each step of the simulation, the segments advance by one unit, $y_i \rightarrow y_i + 1$, with an advancement probability p_i. The p_i depend on the relative positions of the segments, as outlined below.

The p_i are determined by analyzing (qualitatively) the dynamics of superkink motion. Figure 2 contains the three segment configurations which enter the model. (The black dots represent dislocation segments, *not* pinned points.) A segment does not advance if it does not have sufficient edge character. In this simple model, the edge character of a segment is proportional to its slope. A segment is immobile if the magnitude of its slope is less than 2. For this reason, the configurations labeled (a)-(f) are immobile, and $p_i = 0$. The configurations labeled (g) are mobile ($p_i = 1$) because their slope is 2. Configurations (h)-(k) represent pinned segments. A pinning point dissolves when its adjacent segments exert a force larger than a critical dissolution force. The dissolution forces acting on segment i are given by $y_{i+1} - y_i$ and $y_{i-1} - y_i$. If either of these quantities is larger than 2, the pinning point dissolves. The advancement probabilities of configurations (h)-(k) are, therefore, 1. Configurations (l)-(o) represent the upper portion of a superkink. [Any superkink is composed of one configuration selected from the configurations (h)-(k), any number of configurations (g), and a configuration selected from (l) to (o).] The advancement of a segment near the upper edge of a superkink depends on two parameters: the applied stress τ and a parameter reflecting the temperature Θ. The bowing stress, which is proportional to the local circular curvature of the dislocation, opposes the applied stress. The advancement probabilities for configurations (1)-(o) are given by

$$p_i = \max[0, 1 - \Theta/(\tau - \kappa_i)], \tag{7}$$

where κ_i is the circular curvature at segment i, calculated by replacing the appropriate derivatives by their discrete counterparts. Expression (7) reflects the fact that a bowing dislocation moves more slowly, and spends more time in the pinning region [Fig. 1(c)]. The parameter Θ increases with temperature, reflecting the fact that pinning is more frequent.

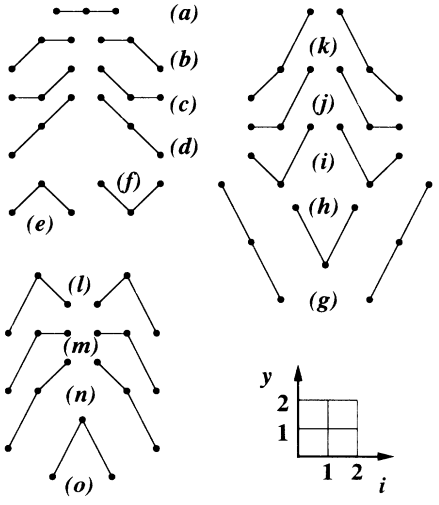

FIG. 2. The three point configurations which enter the model. Each dislocation segment is represented by a solid circle. The advancement probability for the central segment in each configuration depends on the location of its neighboring segments, as described in the text.

The following procedure is used to calculate the exponents. An initial random configuration is generated using the configurations of Fig. 2 labeled (a)-(f). A segment is chosen at random and advanced by one unit. The dislocation advances according to the rules outlined above, until its motion ceases. The advancement time and the total area swept out are recorded, and the process is repeated, starting from the exhausted configuration. In this manner, the distribution of exhaustion events $n(a,t)$ is obtained.

Having obtained the distribution of exhaustion events, it is possible to determine the critical exponents, and, in particular, the creep-rate exponent Δ. In practice, Δ is obtained through the integrated quantities $\tilde{n}(t)$ and $\tilde{n}(a)$,

$$\tilde{n}(t) = \int_0^\infty da\, n(a,t) \text{ and } \tilde{n}(a) = \int_0^\infty dt\, n(a,t). \tag{8}$$

Equation (4) implies that $\tilde{n}(t)$ and $\tilde{n}(a)$ also obey simple power-law relationships. Measurements of their exponents are used to determine the scaling exponents α and δ and, in turn, Δ. It is observed that $\tilde{n}(t)$ and $\tilde{n}(a)$ can be fitted by the Ornstein-Zernike form for the correlation function [9],

$$\tilde{n}(t) \sim t^{-\xi} e^{-t/t_0}, \quad \tilde{n}(a) \sim a^{-\beta} e^{-a/a_0}. \tag{9}$$

The fits produce the exponents required for the calculation of Δ, and also allow estimation of the critical stress through the observed power-law divergences of t_0 and a_0 as a function of the applied stress, τ.

Figure 3 contains the creep-rate exponent calculated as a function of τ for $\Theta = 50$, $L = 100$. The critical stress for these conditions, as estimated from t_0, is $\tau = 100$. The inset of Fig. 3 contains the results obtained from a reanalysis of the data of Thornton, Davies, and Johnston [2]. Note that both the calculation and the experiment have stress-dependent creep-rate exponents that are near 1 over a range of lower stresses. As the stress is increased, the creep-rate exponent decreases to $\Delta \approx \frac{1}{2}$, im-

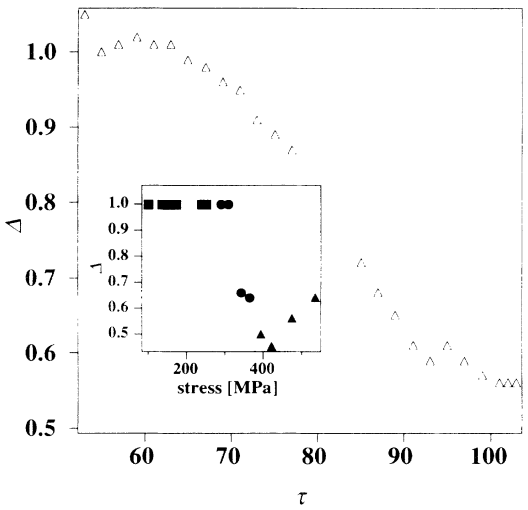

FIG. 3. The creep-rate exponents as a function of applied stress, as predicted by the model, and measured by experiment [2] (the inset). Note that the model accurately reproduces the trend in the creep-rate exponent as measured through experiment. The experimental data were taken at three temperatures: 25 °C (solid squares), 399 °C (solid circles), and 626 °C (solid triangles). The results of the model were obtained for a constant "temperature," $\Theta = 50$, and $L = 100$.

plying a simple power-law dependence on time. The observed variation of the exponents with stress is not completely understood, but may be related to the fact that the system is not always "near" the critical stress. The best estimate of Δ (from the model) at the critical stress is $\Delta = 0.56$ ($\xi = 1.26$ and $\beta = 1.37$). The estimated statistical error in Δ is below 0.01.

It should be noted that Fig. 3 compares the results of experiments performed at three temperatures to the results of the model for one temperature. The authors of Ref. [2] attribute the variation of Δ to a temperature dependence. The model presented here suggests that the variation of Δ stems from the imperfect balance between the thermally assisted pinning of the dislocations and their stress assisted unpinning. The implication is that creep tests performed at constant temperature should display similar trends in the exponents. Further experiments are needed to elucidate this point.

In conclusion, it has been argued that the dislocations in Ni_3Al and related alloys undergo a nonequilibrium phase transition from a phase in which a mobile dislocation ultimately becomes immobile, to a phase in which a mobile dislocation remains mobile for an extended time. The critical exponents of this transition are related, through very general arguments, to creep measurements. It is demonstrated that criticality is the origin of power-law creep rates in Ni_3Al, and suggested that criticality may also explain the power-law creep rates observed in pure metals. A simple model describing dislocation motion yields creep-rate exponents in remarkable agreement, in both qualitative trends and quantitative values, with available experiments.

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