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Microprocesses of the plastic deformation of icosahedral Al–Pd–Mn single quasicrystals

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Abstract

Recent experimental observations on the plastic deformation of icosahedral Al–Pd–Mn single quasicrystals are described originating from conventional transmission electron microscopy in a high-voltage electron microscope (HVEM), from in situ straining experiments in an HVEM and from the determination of activation parameters from macroscopic compression tests at low temperatures. The moving dislocations are created by multiplication events initiated by cross slip. They trail planar faults of different electron microscopy contrast. Since recovery occurs at high temperatures, the dislocation mobility should be discussed on the basis of low-temperature data. While it was previously interpreted in terms of an extended cluster friction model, the present paper shows that it can equivalently be explained by the Peierls mechanism on the cluster scale.

Keywords: Icosahedral quasicrystals; Plastic deformation; Transmission electron microscopy; Peierls model

1. Introduction

After it had become possible to grow large single quasicrystals [1], a dislocation mechanism has been observed to realize the plastic deformation of these materials at high temperatures, first by a drastic increase of the dislocation density after deformation [2], and later on by the direct observation of the dislocation motion during in situ straining experiments in a high-voltage electron microscope (HVEM) [3]. The activation parameters of the plastic deformation of icosahedral Al–Pd–Mn single quasicrystals were first determined in [4] and attributed to the friction mechanism of dislocations. More detailed measurements showed that a continuous plastic deformation of Al–Pd–Mn quasicrystals is only possible if recovery compensates the strong work-hardening during loading [5,6] so that the intrinsic friction mechanism of dislocations should be studied at the lowest possible temperatures. This paper presents new results on the microstructure at a relatively low deformation temperature, the dislocation generation and the deformation parameters. The results are discussed in terms of dislocation models.

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2. Results

The microstructure of icosahedral Al–Pd–Mn single quasicrystals was studied in an HVEM, which, due to its large penetration depth, allows a good imaging of the spatial arrangement of the dislocations. After deformation at 610°C, the dislocations are either distributed quite homogeneously as in Fig. 1a, or they are concentrated in narrow slip bands. The dislocation densities amount to about $10^{12}\,m^{-2}$ in the homogeneous regions, and to $1.3\times10^{13}\,m^{-2}$ in the centre of the bands.

Stereo pairs reveal that many dislocations are arranged in more than one distinct plane, suggesting that cross slip frequently occurs. The latter is a prerequisite to a cross slip multiplication mechanism for generating new dislocations during deformation. Characteristic intermediate configurations of such a mechanism are frequently observed as, e.g. the α-like one in Fig. 1a, with a new loop L forming at an immobile jog J. Fig. 2 presents sections of a video record of a multiplication event observed during in situ straining in an HVEM. A dislocation extends to the right in (a), acquires a jog J in (b), the cross slipped segment extends to a loop L in (c), when the lower part of the loop emerges through the surface, the loop splits into two dislocations moving in opposite directions in (d). Thus, the new experiments show that new dislocations are

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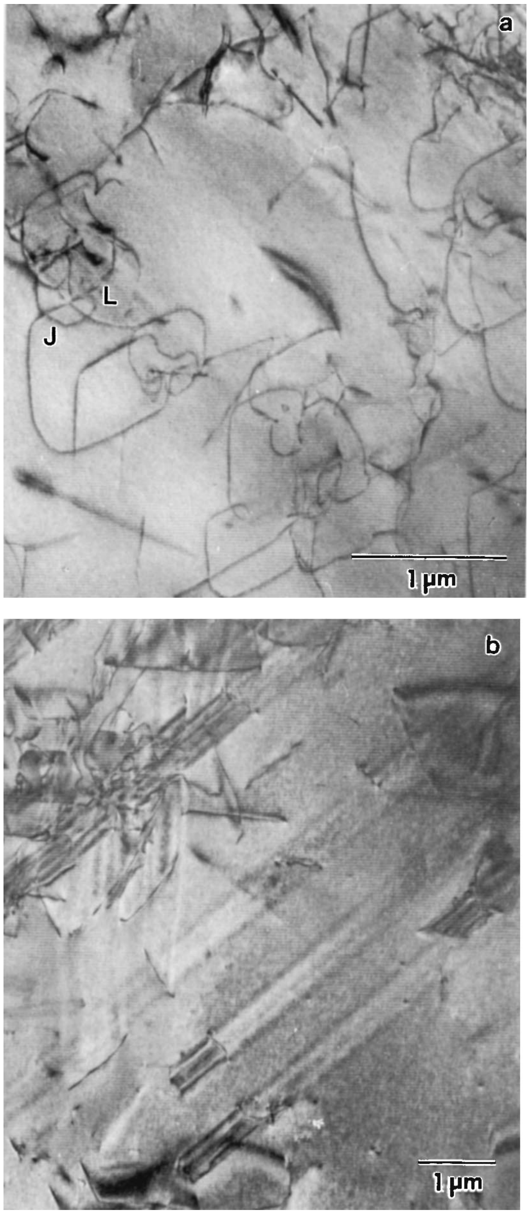

Fig. 1. Dislocation structures after 0.7% plastic deformation at 610°C, (a) homogeneous distribution of dislocations; (b) dislocations and planar faults of different contrast.

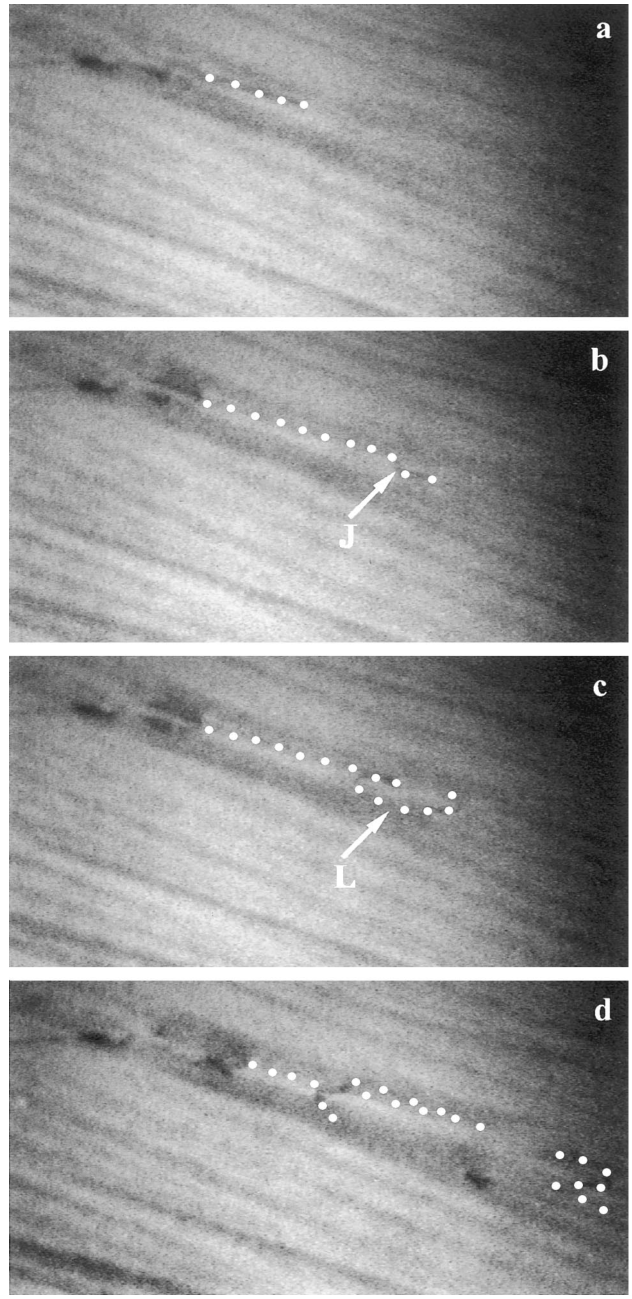

Fig. 2. Sections of a video sequence of a multiplication event during in situ deformation at 675°C.

created during the deformation of quasicrystals by a cross slip mechanism.

It has been pointed out before that during in situ experiments the dislocations move in a viscous way and are arranged in preferred crystallographic directions [3,7]. This arrangement is conserved even in the micrographs taken in a relaxed state as, e.g. in Fig. 1a. However, the dislocations are not totally straight but are curved especially at the corners between the almost straight segments. The radius of curvature δ at the corners varies between about 0.15 and 0.5 µm.

Many dislocations trail planar faults with clear fringe contrast as shown in Fig. 1b. The strong fringe contrast is frequently bound by dislocations. Some times weak fringes appear outside the area of strong contrast and mark the trail of the dislocation over a longer distance. Micrographs like Fig. 1b demonstrate that planar faults of different structure are produced behind moving dislocations.

A full set of parameters of the steady state deformation at strain rates of 10^{-5} and $10^{-4}\,s^{-1}$ is published in [5] and discussed in [6]. At $10^{-5}\,s^{-1}$, the specimens become brittle below about 630°C. To obtain deformation data below that temperature, specimens were deformed down to 500°C at a rate of $10^{-6}\,s^{-1}$ with stress relaxation tests already during the quasi-elastic loading, as briefly mentioned in [7] and

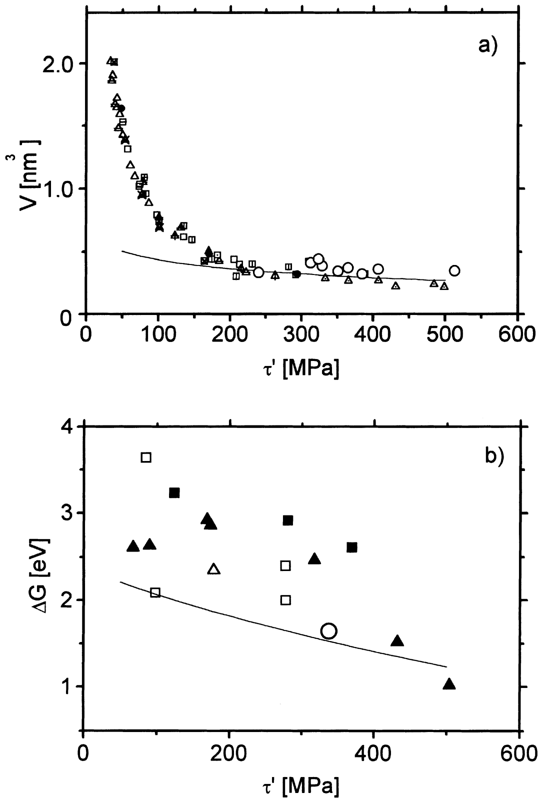

Fig. 3. Activation volume V from stress relaxation tests, corrected for work-hardening, (a) and Gibbs free energy ΔG (b) as a function of the normalized stress τ'. Small symbols: data from high-temperature steady state deformation after [6]. Open circles: data from low-temperature tests. Full lines: prediction of the Peierls mechanism.

described in more detail in [8]. Within this low-temperature range, the specimens show a very strong work-hardening with hardening coefficients of the order of Young's modulus. As the hardening occurs also during the stress relaxation tests, the strain rate sensitivity data obtained from these tests have to be corrected for the hardening. Fig. 3a shows a plot of the activation volume from stress relaxation tests versus a normalized stress $\tau'=\mu_0 m_s \sigma/\mu(T)$, where μ_0 is the shear modulus at zero temperature, m_s the orientation factor set equal to 0.4, σ the actual (technical) stress, and $\mu(T)$, the shear modulus at the temperature T (μ=68 GPa at 610°C). The major part of the data refers to the high-temperature steady state deformation and originates from [6]. The new low-temperature data are plotted as larger open circles. They show activation volumes slightly larger than those of the steady state deformation. A single value of the Gibbs free energy of activation has been determined up to now. Fig. 3b shows that it is lower than the values of the steady state deformation at equal stress τ'.

3. Discussion

It is argued in [6] that the steady state deformation of quasicrystals is only possible if recovery compensates the strong work-hardening. Hence, the high-temperature data of all previous measurements ([4,5] and others) have to be interpreted by using the standard theories of high-temperature deformation as discussed in [8]. However, the low-temperature results presented here and in [8] should allow conclusions to be drawn on the intrinsic deformation mechanisms of quasicrystals. They will be discussed in the following.

At all temperatures, an important contribution τ_i to the flow stress τ should result from long-range dislocation interactions. In [6], for the high-temperature range τ_i was estimated from the dislocation densities ρ from [9], using the relation for Taylor hardening,

$$\tau_i = \alpha \mu b \rho^{1/2} \tag{1}$$

with $\alpha \cong 0.5$, and b, the length of the Burgers vector in physical space (most frequent value b=0.183 nm, e.g. [10]). The dislocation densities observed in [9] are quite high leading to a remarkable contribution of τ_i to the relatively low flow stresses at high temperatures. The values of ρ described above for 610°C are at least one order of magnitude smaller leading to τ_i=7–25 MPa, only, compared to τ of the order of 400 MPa. This contradicts the strong work-hardening observed particularly at low temperatures. This and the disagreement between the present dislocation densities and those of [9] at higher temperatures remain open problems.

The new micrographs of the present study show that dislocations frequently trail planar faults as in Fig. 1b. The faults with strong contrast may be stacking faults trailed by partial dislocations but at least those of weak contrast should be phason layers as predicted by the theory and computer simulation experiments [11]. A thorough contrast analysis is necessary to characterize these faults in more detail. In [12], the (athermal) friction stress τ_{ph} owing to the trailing of the phason layers was estimated at τ_{ph}=54 MPa based on the theoretical results of [11]. Unfortunately, the present micrographs do not give information on the friction stress of the faults.

The curved dislocation segments at the corners of the straight branches in the unloaded state of the dislocation structures as shown, e.g. in Fig. 1a, cause a back stress, which is balanced by a velocity-dependent friction stress τ_{fr}. As the unloading and cooling to a sufficiently low temperature took about 15 min, τ_{fr} should correspond to a low velocity. τ_{fr} can be estimated from the radius of curvature δ by the line tension theory

$$\tau_{fr} = \frac{\Gamma}{(b\delta)} \tag{2}$$

with $\Gamma=\mu b^2/(4\pi)$ ln $[2\delta/(5b)]$ being the line tension. Using the values of δ quoted above, τ_{fr} amounts to only 15–40 MPa. It will be higher for higher dislocation velocities.

Up to now, the plastic deformation data of quasicrystals have mainly been discussed on the basis of the friction mechanism of dislocations. Urban and coworkers (e.g. [10]) proposed that the friction stress τ_{fr} is controlled by overcoming the strongly bound Mackay-type clusters. This mechanism has been discussed in a more quantitative way by considering the clusters to be weak obstacles, which leads to an agreement with the activation volumes measured [12]. Also in this extended version, the model cannot explain the strong decrease of the flow stress of Al–Pd–Mn quasicrystals with increasing temperature above about 640°C. As mentioned above, this decrease is now interpreted by recovery [6]. An alternative approach to the cluster friction mechanism may be the Peierls mechanism as first proposed in [13]. Considering the cluster structure of the quasicrystals, it may be scaled up to the larger scale of the Mackay-type clusters as suggested in [14]. Their diameter and the Peierls stress τ_p at zero temperature determine the Peierls energy as well as the kink formation energy G_k [12]. The Peierls mechanism explains naturally the oriented shape of dislocations occurring in the present micrographs as well as during the dislocation motion in the in situ experiments [3,7]. For this mechanism, the Gibbs free energy of activation may read as [15]

$$\Delta G(\tau) = 2G_k \left[1 - \frac{\pi\tau}{(8\tau_p)}\left\{\ln\left[\frac{16\tau_p}{\pi\tau}\right] + 1\right\}\right] \tag{3}$$

This function is plotted in Fig. 3b using τ_p=1.5 GPa and G_k=1.2 eV. Fig. 3a shows the dependence of V on the stress considering that $V=-\mathrm{d}\Delta G/\mathrm{d}\tau$. Both functions are consistent with the experimental data at low temperatures, i.e. at high stresses. As discussed above, recovery leads to different parameters at high temperatures.

4. Conclusions

The following conclusions can be drawn:

- At low temperatures, Al–Pd–Mn single quasicrystals show a strong work-hardening implying a large athermal stress contribution. The required high dislocation densities have not yet been observed.
- Dislocation multiplication may occur by a cross slip mechanism.
- Planar faults are trailed by moving dislocations. Up to now, there is no experimental information in which way they contribute to the flow stress.
- The dynamic friction stress of dislocations, which is not very high at low temperatures, can equivalently be explained by the extended cluster friction model and by the Peierls mechanism on the scale of clusters.

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