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Friction mechanism of dislocation motion in icosahedral Al–Pd–Mn quasicrystals

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ABSTRACT

Results from the literature and unpublished ones of the present authors are summarized which are relevant to the mechanisms governing the mobility of dislocations in icosahedral Al–Pd–Mn quasicrystals. These results concern macroscopic deformation tests, conventional transmission electron microscopy, *in situ* straining experiments in a transmission electron microscope, and computer simulation experiments. These experiments can best be interpreted by assuming that the dislocation motion is controlled by the thermally activated overcoming of Mackay-type clusters. The present paper gives an estimate of the activation volume of this process. It turns out that the activation volume of overcoming the clusters individually is one order of magnitude smaller than the experimentally observed one. The experimental observations can be interpreted in a consistent way in terms of the Labusch–Schwarz theory of solution hardening in crystals, which considers the interpenetrating clusters as 'extended' obstacles, a number of which are surmounted collectively. Some implications of this new model are discussed.

§ 1. INTRODUCTION

Quasicrystals are brittle at low temperatures but can be deformed plastically at high temperatures. This was shown for icosahedral Al–Pd–Mn single quasicrystals by Wollgarten *et al.* (1993) and by Inoue *et al.* (1994). The intrinsic macroscopic deformation parameters were determined by Feuerbacher *et al.* (1995) for Al–Pd–Mn single quasicrystals. During deformation, the dislocation density increases strongly, pointing to the operation of a dislocation mechanism (Wollgarten *et al.* 1993). This conclusion has been confirmed by Wollgarten *et al.* (1995) by the direct observation of moving dislocations during *in situ* straining experiments in a high-voltage electron microscope. These experiments showed that the dislocations move in a viscous way. On the basis of this observation and taking into account the macroscopic deformation parameters, Feuerbacher *et al.* (1997) and Urban *et al.* (1998) suggest that the interaction with the Mackay-type clusters occurring in the quasicrystal lattice provides the basic friction mechanism of mobile dislocations, thus controlling the rate of macroscopic plastic deformation. The present paper

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discusses this mechanism in more detail and shows that the theory by Labusch and Schwarz (1991) of overcoming 'extended' obstacles can be applied to the cluster friction model yielding quantitative agreement with most of the experimental results. The basic experimental and theoretical observations relevant for a discussion of dislocation friction in quasicrystals are briefly outlined in § 2. The model is described in § 3 followed by a discussion in § 4.

§ 2. Experimental observations and results of computer simulations

2.1. *Macroscopic deformation*

Macroscopic deformation tests were performed in compression at strain rates of 10^{-5} and $10^{-4}\,s^{-1}$ along twofold quasicrystal axes by Feuerbacher *et al.* (1995) and Geyer *et al.* (1998) and along fivefold axes by Brunner *et al.* (1997) and Geyer *et al.* (1998). According to the latter study, the deformation parameters depend on the compression direction only weakly.

The results of the deformation tests on quasicrystals were discussed in terms of the models of dislocation motion in crystals, where the strain rate $\dot{\varepsilon}$ is given by an Arrhenius-type relationship (for a review see, for example, Evans and Rawlings (1969))

$$\dot{\varepsilon}(\tau, T) = \dot{\varepsilon}_0 \exp(-\Delta G(\tau)/kT). \quad (1)$$

The same approach is used in the present paper. The pre-exponential factor $\dot{\varepsilon}_0$ depends on the mobile dislocation density and is considered constant during the measuring procedures of the activation parameters. ΔG is the Gibbs free energy of activation, which is a function of the shear stress τ, k is Boltzmann's constant, and T is the absolute temperature. The 'experimental' activation volume $V_{ex} = kT/m_s r$ was calculated from the strain rate sensitivity $r = (\Delta\sigma/\Delta \ln \dot{\varepsilon})_T$. Here, σ is the flow stress and m_s is the orientation factor. As shown below, $m_s \cong 0{\cdot}4$. The macroscopic data of Geyer *et al.* (1998) cover the widest temperature range available at present. Therefore, the following discussion is based on these data. The strain rate sensitivity was determined mainly from stress relaxation tests. Between about 640°C and 830°C, the flow stress at $\dot{\varepsilon} = 10^{-5}\,s^{-1}$ decreases from values above 800 MPa down to less than 100 MPa. At the same time, the strain rate sensitivity r decreases from a rather constant value of about 140 MPa between 640°C and about 680°C down to about 25 MPa at 830°C. This corresponds to an increase of the experimental activation volume from about 0.25 up to 1.5 nm^3.

In equation (1), the strain rate is controlled by the Gibbs free energy of activation ΔG. Unfortunately, this quantity is not directly accessible in the experiments. Instead, the activation enthalpy $\Delta H = -kT^2(\Delta\sigma/\Delta T)/r$ was calculated from the temperature sensitivity of the flow stress $(\Delta\sigma/\Delta T)$ at a constant strain rate. The ΔH values increase from about 2 eV at 640°C up to about 4.4 eV at 735°C. Reliable data of ΔH characterizing the dislocation mobility cannot be determined for higher temperatures because of recovery, as discussed below. For crystals, the Gibbs free energy of activation $\Delta G = \Delta H - T\Delta S$ is usually calculated from ΔH using an equation derived by Schöck (1965). ΔS is the activation entropy, which is estimated on the assumption that entropy terms arise solely from the temperature dependence of the elastic moduli. Applying this formalism also to quasicrystals and using the data by Tanaka *et al.* (1996) for the temperature dependence of the shear modulus yields ΔG values increasing from about 1 eV at 640°C up to 2.3 eV at 735°C.

A number of observations indicate that the long-range athermal component of the flow stress is small and that recovery plays an important role in the deformation behaviour of quasicrystals, particularly at high temperatures. This concerns the following observations.

(a) During long-time stress relaxation tests, the flow stress drops to very small values.

(b) Stress dip tests at 760°C show zero relaxation at about 20% of the flow stress, and back-flow at lower stresses (Feuerbacher 1996).

(c) The original relaxation curves and the curves obtained from repeating the relaxation tests after re-loading the specimens up to stresses smaller than the starting stresses of the original relaxations do not coincide, particularly at high temperatures (Geyer *et al.* 1998). The repeated relaxation curves show smaller strain rates (which are proportional to the negative stress rates) at the same stresses and therefore yield higher strain rate sensitivities than the original relaxation curves. The decrease of the strain rate can be explained by recovery of the dislocation density during the first relaxation. After relaxation, the original dislocation density is only restored when some plastic strain has evolved. Then, a yield point effect appears, the height of which is in agreement with the reduction of the mobile dislocation density during the first relaxation.

2.2. *Microscopic observations*

The dislocations move on well-defined slip planes, which is concluded from analysing the Burgers vector and dislocation line directions by conventional transmission electron microscopy (Rosenfeld *et al.* 1995) and from *in situ* straining experiments in a high-voltage electron microscope (Wollgarten *et al.* 1995, Messerschmidt *et al.* 1998). According to these studies, the planes perpendicular to fivefold, threefold, twofold, and pseudo-twofold directions are the most frequent slip planes. The parallel components of the most frequent Burgers vectors lie along twofold directions (Rosenfeld *et al.* 1995). Considering the most frequent slip planes and directions as well as the high degree of isotropy of the quasicrystals, usually leading to multi-slip, $m_s \cong 0{\cdot}4$ seems to be a good estimate of an average orientation factor. With increasing strain, the ratio between the phason and phonon components of the six-dimensional Burgers vectors of dislocations increases.

The stress–strain curves of icosahedral Al–Pd–Mn quasicrystals exhibit a pronounced yield drop phenomenon. During loading up to the lower yield point, the dislocation density increases by more than two orders of magnitude and decreases at larger strains (Wollgarten *et al.* 1993, Feuerbacher *et al.* 1997). The dislocation density at constant plastic strain (1.3%) measured on samples rapidly quenched after deformation decreases from $9 \times 10^{13}\,\mathrm{m}^{-2}$ at 695°C to $3 \times 10^{12}\,\mathrm{m}^{-2}$ at 820°C (Schall *et al.* 1998). From the dislocation density ρ, the long-range athermal component of the flow stress τ_i can be estimated using the well-known formula for Taylor hardening (Taylor 1934)

$$\tau_i = 0{\cdot}5\mu b\rho^{1/2}, \tag{2}$$

where μ is the shear modulus and b is the modulus of the Burgers vector. With $\mu \cong 50$ GPa (Tanaka *et al.* 1996), $b = 0{\cdot}183$ nm (the most frequently observed length of the Burgers vector component in physical space) and the dislocation densities quoted above, τ_i turns out to amount to only about 5% of the total flow stress. For dislocation densities even five times larger during deformation (i.e. taking possible recovery processes into consideration), the athermal component of the flow stress would still be small, agreeing well with the result of the dip tests mentioned above. Annealing a specimen at 730°C previously deformed at the same temperature reduces the dislocation density (Schall *et al.* 1998). The half-time of this process is only about 10 min, which emphasizes the importance of recovery even at this relatively low temperature.

The *in situ* straining experiments in a high-voltage electron microscope at temperatures between 700 and 750°C have shown that the dislocations move in a steady viscous way (Wollgarten *et al.* 1995, Messerschmidt *et al.* 1998). Dislocations on different slip systems move at different velocities. Figure 1 shows that under load the dislocations mostly are of angular shape with straight segments in preferential orientations. The preferred orientations determined so far are parallel to twofold directions on a threefold slip plane, and to an orientation inclined about 60° to the twofold direction on a pseudo-twofold plane (Messerschmidt *et al.* 1998). The angu-

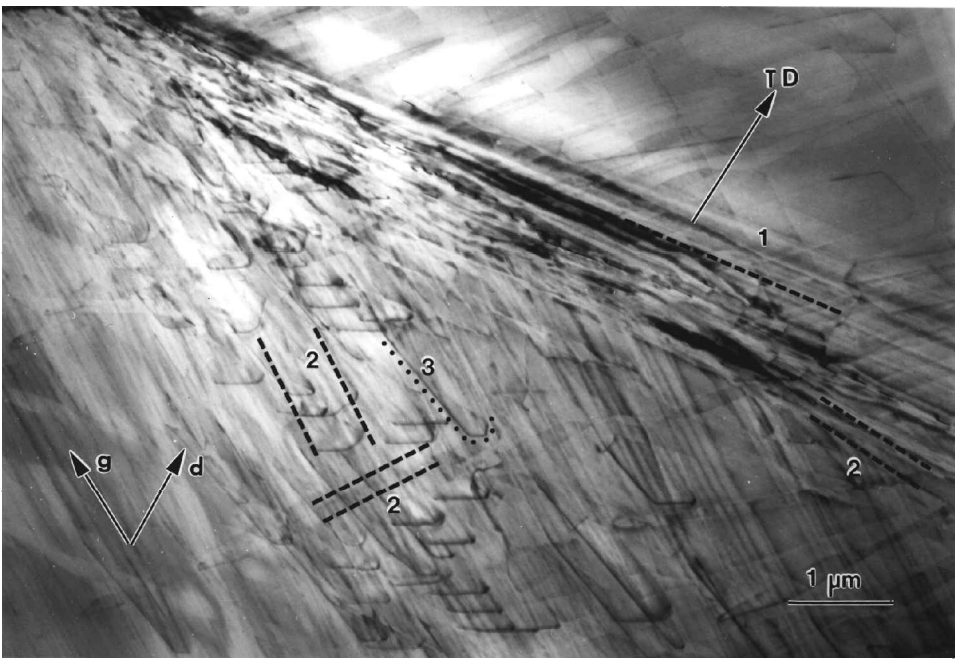

Figure 1. Dislocations moving during *in situ* straining in a high-voltage electron microscope at about 750°C. Tensile direction TD near to a twofold direction, beam direction in threefold direction. The normal of the foil plane is tilted by about 15° with respect to the beam direction. *g*-vector: $g = [1/0\ 1/1\ 0/1]$, $d = [0/1\ 1/0\ 1/1]$. Dashed lines: traces of slip planes: (1) plane perpendicular to a twofold direction imaged almost edge-on, (2) different planes perpendicular to threefold directions, the widths of the traces of the slip planes are indicated. All dislocations are arranged perpendicular to twofold directions. The three twofold directions on a threefold plane are marked by a dotted line (3).

lar shape of dislocations was not observed by *post mortem* electron microscopy of deformed material (Rosenfeld *et al.* 1995). It should be pointed out that all results on the dislocation structure originate from deformation tests at or above 730°C, except the *in situ* experiments performed at 700°C. The dislocation arrangement observed under these conditions may have been influenced by recovery and need not represent the situation at low deformation temperatures. Nevertheless, it seems quite clear that a great part of the flow stress of Al–Pd–Mn single quasicrystals is controlled by an intrinsic friction mechanism of moving dislocations, the density of which strongly depends on the deformation conditions.

2.3. *Results of computer simulation studies*

There is a number of studies in which the motion of dislocations in two- and three-dimensional quasi-periodic structures is investigated by computer simulation. The results of molecular statics calculations indicate that the dislocations glide on well-defined planes, producing a layer of a high concentration of phason defects along their glide plane (Dilger *et al.* 1997, Takeuchi *et al.* 1998) as well as isolated phason defects (Takeuchi *et al.* 1998). In a three-dimensional simulation, the energy of the phason layers was estimated to be 58% of the surface energy (Dilger *et al.* 1995). In two-dimensional molecular dynamics simulations at 10^{-6} of the melting temperature (Mikulla *et al.* 1998), a dislocation placed on a plane between densely packed planes was observed to dissociate into partial dislocations at a stress of $0{\cdot}02\mu$. Individual partial dislocations have been observed experimentally (Rosenfeld *et al.* 1995), but no split dislocations of small width. In the simulation, both partials started to move at a shear stress of $\tau_0 = 0{\cdot}03\mu$. In Al–Pd–Mn this corresponds to a shear stress of 1.5 GPa, which may be considered a theoretical estimate of the friction stress close to 0 K. In the calculations, the dislocations were observed to stop in front of local configurations of high coordination, the structure of which has been identified in the two-dimensional models. Analogous structures for the three-dimensional case have not yet been specified. At low temperatures, the layers of phasons, produced by the gliding dislocations, remain flat but at high temperatures the phasons diffuse away to form a wide damaged zone (Mikulla *et al.* 1996).

§ 3. Model of dislocation friction in quasicrystals

As shown by Boudard *et al.* (1992), the structure of icosahedral Al–Pd–Mn quasicrystals can be described either as a quasi-periodic arrangement of two types of Mackay-type clusters or as the stacking of densely and less densely packed planes. Both views are important for the understanding of the mechanism of dislocation motion. The Mackay-type clusters are strongly bound structural units with a diameter of about 0.9 nm, consisting of a central Mn atom, a core consisting of 8 Al atoms, an inner icosahedron of either Mn and Al or Mn and Pd atoms and an outer icosidodecahedron of Pd and Al atoms or Al atoms only, which Boudard *et al.* (1992) termed pseudo-Mackay clusters of type 1 and 2, respectively. Perfect Mackay-type clusters comprise about 60% of the atoms, while the rest of the atoms, between the clusters, are arranged in patterns which can be considered to be related to incomplete clusters. The investigation of cleavage surfaces of Al–Pd–Mn quasicrystals by means of scanning tunnelling microscopy demonstrates that the clusters are mechanically highly stable. Complete clusters are preserved at the surface, which shows that cracks circumvent the Mackay-type clusters, which therefore

have to be considered rigid obstacles capable of deflecting propagating cracks (Ebert *et al.* 1996).

The centres of the clusters are arranged along crystallographic directions on crystallographic planes. This is demonstrated in figure 2, which is plotted after the data of Boudard *et al.* (1992), for the twofold directions on planes perpendicular to a fivefold axis. Between the densely packed planes containing the centres of clusters, there are planes of low packing density, which are not shown in the work by Boudard *et al.* but between which the dislocations most probably glide (Yang *et al.* 1998). This assumption was made also by Mikulla *et al.* (1998). The spacing between the planes packed with cluster centres certainly never exceeds 0.6 nm. This means that the slip planes cut at least the outer shells of the Mackay-type clusters.

It was suggested by Feuerbacher *et al.* (1997) and Urban *et al.* (1998) that these Mackay-type clusters act as obstacles to the dislocation motion, and that the resulting friction controls the plastic deformation. This mechanism was termed a cluster friction model by the authors. The main argument supporting this view is that the experimental activation volume V_{ex} ranging from 0.25 to 1.5 nm^3 depending on the deformation conditions applied, which corresponds to $40b^3$ to $245b^3$, is considerably larger than a few b^3, which would be expected for the lattice friction mechanism (Peierls mechanism) in crystals. Thus, the dislocation mobility should be controlled by items of a larger length scale than double kinks forming along a dislocation line in crystals. The mutual distance as well as the size of the Mackay-type clusters fit this

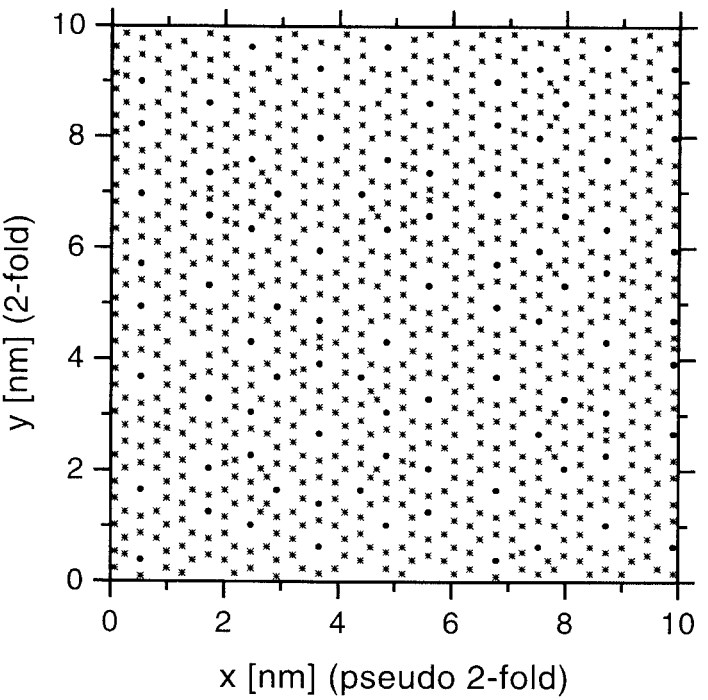

Figure 2. Atomic arrangement in a plane perpendicular to a fivefold axis (from a data set generated by Boudard *et al.* (1992)). *: Al atoms; •: Mn atoms. Rings of 10 Al atoms around a Mn atom arranged along twofold directions characterize the Mackay-type clusters.

length scale. It is the aim of the present paper to work out the cluster friction model in more detail.

According to the above discussion it is most probable that the Mackay-type clusters are not cut near their equators but along planes of low packing density between the planes of cluster centres. Owing to the relation between the diameters and the distances between the clusters, their outer shells have to be cut in any case, and it is probably these events that control the dislocation motion. This implies that the dislocations will arrange parallel to orientations of a high cluster density. As pointed out above, *in situ* experiments revealed preferred orientations of the dislocations. As described in § 2.3, there may also be hard spots along the slip planes other than some features of the Mackay-type clusters, like those identified by Mikulla *et al.* (1998) in the two-dimensional simulations. To the authors' knowledge, however, to date, no corresponding result of calculations of a three-dimensional structure has been obtained. It is expected that the distances between these other hard spots will be of the same order of magnitude as those between the centres of the Mackay-type clusters as they are on the same level of the structure hierarchy.

According to the model of the thermally activated overcoming of individual localized obstacles in crystals, the activation volume is given by (see, for example, Evans and Rawlings (1969))

$$V_{ind} = ldb, \tag{3}$$

where l is the obstacle distance along the dislocations, and d is the so-called activation distance. The latter is the distance, shown in figure 3, in forward direction along the force–distance profile of the dislocation interaction between the stable equilibrium configuration y_e in front of the obstacle and the respective labile one y_l where the dislocation leaves the obstacle, $d = y_l - y_e$. Both l and d decrease with increasing shear stress. The area $A = ld$ is also called the activation area. This is the area swept by the dislocation during the activation event. The situation is schematically shown in figure 4 for cutting the clusters near their equators. An upper limit of V_{ind} can be estimated in the following way. According to Boudard's structure model, the distances between the centres of the Mackay-type clusters are of the order of 1 nm. For example, in the fivefold planes the shortest distances are $l_1 = 0.78$ nm and

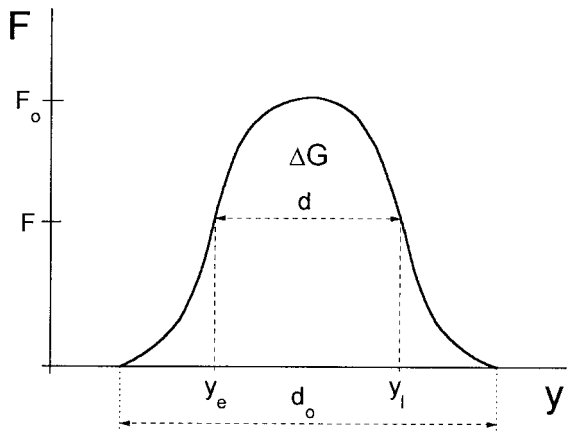

Figure 3. Force–distance curve of the interaction between a dislocation and a localized obstacle.

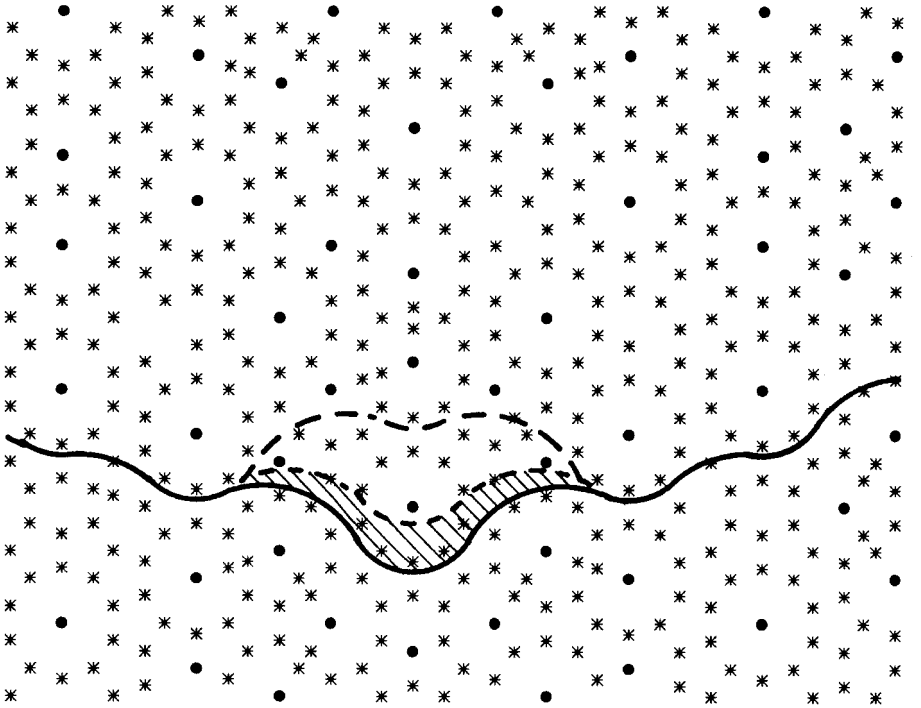

Figure 4. Schematic drawing of a dislocation bowing out between Mackay-type clusters. The arrangement of atoms is a section of figure 2. In the figure, it is assumed that the clusters are cut near their centres. The hatched area is the activation area of overcoming a single obstacle.

$l_2 = \tau l_1 = 1{\cdot}26\,\mathrm{nm}$. Here, $\tau = (5^{1/2} + 1)/2$ denotes the number of the golden mean. Thus, assuming $l \cong 1\,\mathrm{nm}$ for the obstacle distance should represent a reasonable estimate. l would be smaller by a factor of $2^{1/2}$ if it were considered that the clusters from both sides intersect the slip plane. The value of d at zero stress d_0 depends on the shape of the interaction profile and is usually a fraction of the diameter of the obstacle. Figure 4 shows a dislocation in the equilibrium position waiting for thermal activation as a full line, and after having overcome the central obstacle as a dotted line. The hatched area between both configurations is the corresponding activation area A. The cluster diameter is certainly an upper bound of the activation distance, so that $d_0 = 0{\cdot}9\,\mathrm{nm}$. With these data, the maximum value of the activation volume of overcoming individual clusters should be of the order of magnitude of $V_{ind\,0} = 1 \times 0{\cdot}9 \times 0{\cdot}183\,\mathrm{nm}^3 \cong 0{\cdot}16\,\mathrm{nm}^3$. In principle, d_0 might also be much larger than the obstacle diameter. However, the area per obstacle, which is equal to l^2, is an ultimate upper limit of the activation area. In figure 4, this area is limited by the full and dashed lines, and it leads to an almost equal estimate of $V_{ind\,0}$. If the clusters are not cut at their equators, which is supposed here, d_0 as well as $V_{ind\,0}$ should be considerably smaller. $V_{ind\,0}$ has to be compared with the largest experimental value of $V_{ex} = 1{\cdot}5\,\mathrm{nm}^3$. This value corresponds to small stresses or high temperatures. As discussed in §2.1, it may be influenced by recovery, but not by an order of magnitude. Thus, the experimental activation volume V_{ex} determined from the strain rate sensitivity of the flow stress is at least one order of magnitude larger than the

activation volume V_{ind0} of overcoming the Mackay-type clusters individually. At increasing stress (or decreasing temperature), the experimental activation volume decreases but the mismatch between the model and the experimental value remains unchanged.

The model of overcoming the Mackay-type clusters as individual localized obstacles treated so far does not reflect the nature of the quasicrystal structure, where the individual clusters penetrate each other. A better description of the dislocation motion may be obtained by the theory of Labusch and Schwarz (1991) for so-called 'extended' obstacles. This theory was derived for solution hardening in crystals where a relatively rigid dislocation moves in the field of weak obstacles. In this case, the dislocation changes its position not only at and near an obstacle which is overcome by an event of thermal activation, but also at a number of neighbouring obstacles. The theory has to be applied if the width of the obstacle profiles is not small compared to the bow-out of the dislocation segments between the obstacles. According to Labusch and Schwarz (1991), this criterion is fulfilled if the normalized obstacle width, defined by

$$\eta_0 = d_0(2\Gamma c/F_0)^{1/2}, \tag{4}$$

is not small with respect to unity. c is the concentration of obstacles on the slip plane, which is given by $c \cong l^{-2}$. F_0 is the maximum force the obstacles can sustain and Γ is the dislocation line tension. It is approximated here by $\Gamma = \mu b^2/2 = 8{\cdot}4 \times 10^{-10}$ N with the shear modulus $\mu \cong 50$ GPa at high temperature as quoted above. F_0 is unknown. According to the theory of Labusch and Schwarz (1991), there is a relation between F_0, the obstacle concentration c and the athermal flow stress of the obstacle array,

$$\tau_0 = 0{\cdot}94(1 + 2{\cdot}5\eta_0)^{1/3}F_0^{3/2}(c/2\Gamma)^{1/2}/b. \tag{5}$$

As described in §2, a theoretical estimate of the athermal flow stress is $\tau_0 = 0{\cdot}03\mu = 1{\cdot}5$ GPa. This seems to be a realistic estimate as it is about five times the maximum flow stress ($\sigma = 800$ MPa corresponding to $\tau = 320$ MPa) at the lowest temperature of the experiments. Using this value and the above estimates of c, Γ and d_0, equations (4) and (5) can be solved simultaneously to yield $\eta_0 = 1{\cdot}97$ and $F_0 = 3{\cdot}52 \times 10^{-10}$ N. $d_0 = 0{\cdot}9$ nm is certainly too large for cutting the clusters off-centre. A smaller and more realistic value of $d_0 = b = 0{\cdot}183$ nm results in $\eta_0 = 0{\cdot}35$ and $F_0 = 4{\cdot}54 \times 10^{-10}$ N. In both cases, however, η_0 is well in the range of application of the theory of Labusch and Schwarz (1991) so that the situation of cutting Mackay-type clusters should be described by the theory of overcoming 'extended' obstacles.

The theory implies that the activation volume V_{ex} determined macroscopically from the strain rate sensitivity can be larger than that of surmounting individual obstacles by several orders of magnitude. This is shown in figure 5, where the normalized experimental activation volume V_{ex}/V_0 is plotted versus a normalized temperature T/T_0. The normalizing constant of the activation volume is given by

$$V_0 = bg\eta_0/c, \tag{6}$$

and that of the temperature by $T_0 = \Delta G_0/(k \ln(\dot{\varepsilon}_0/\dot{\varepsilon}))$. g is a factor depending on the shape of the interaction potential, which is close to unity. Using the data discussed above yields a value for V_0 of the order of magnitude of 0.1 nm^3. Thus, V_{ex}/V_0 is about 10 and $T/T_0 \cong 2{\cdot}5$ follows from figure 5. The ratio of T/T_0 equals

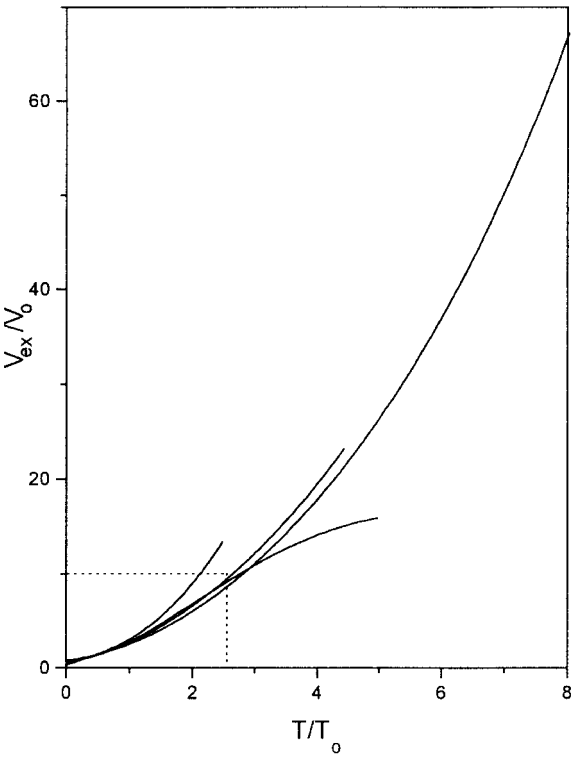

Figure 5. Dependence of the normalized experimental activation volume V_{ex}/V_0 on the normalized temperature T/T_0 after the theory of overcoming extended obstacles. Re-plotted from the paper of Labusch and Schwarz (1991).

the ratio between the experimental activation energy ΔG_{ex} and the activation energy of surmounting individual obstacles ΔG_{ind}

$$T/T_0 = \Delta G_{ex}/\Delta G_{ind}. \tag{7}$$

Thus, the energy barrier to overcome an individual cluster is certainly smaller than the respective values observed in the experiments.

§ 4. Discussion

The present paper gives an estimation of the activation volume of the cluster friction model established by Feuerbacher *et al.* (1997) and Urban *et al.* (1998). The microprocesses during the thermally activated events are still not clear. As described above, the clusters are most probably cut off-centre along planes of large distances. Molecular dynamics simulations in three dimensions similar to the two-dimensional ones by Mikulla *et al.* (1998) may help to identify the atomic configurations acting as obstacles. Nevertheless, these configurations will be of the size and spacing of the Mackay-type clusters in the structural hierarchy of quasicrystals, whatever their exact atomic structure.

The estimations of § 3 show that the maximum value of the activation volume of overcoming individual clusters is about one order of magnitude smaller than the maximum volume measured in macroscopic deformation tests. This discrepancy can be overcome if the obstacles are considered to be extended obstacles in the sense of

the theory by Labusch and Schwarz (1991). The theory predicts that at high temperatures the obstacles are not surmounted individually but that in a thermally activated event the dislocation is shifted at a number of obstacles. Consequently, the activation energy controlling dislocation glide is larger than that of an individual obstacle, and at the same time the dislocation sweeps a larger area during the activation. Thus, a combination of the cluster friction and the extended obstacle models can explain the large values of the experimental activation volume.

According to equation (7) and figure 5, the fact that V_{ex}/V_0 is about 10 implies that the experimental Gibbs free energy of activation ΔG_{ex} should be about 2.5 times larger than the value ΔG_{ind} of the individual obstacles. The same conclusion can be drawn from figure 4 of the paper by Labusch and Schwarz (1991) considering that the experimental stress range is below one fifth of the maximum stress τ_0. As described in § 2.1, in the experiments quite large activation enthalpies are observed. Using the data of Geyer *et al.* (1998), the formalism for crystals of Schöck (1965) and the temperature dependence of the shear modulus according to Tanaka *et al.* (1996) yielded ΔG values of 1 eV at 640°C and of 2.3 eV at 735°C. Reasonable values of ΔG, i.e. values corresponding to a reasonable pre-exponential factor $\dot{\varepsilon}_0$ in equation (1), amount to about $25kT$, which is about 2 eV at 640°C and 2.2 eV at 735°C. This means that the experimental values are of a reasonable order of magnitude. According to figure 5, the Gibbs free energy ΔG_{ind} to overcome the individual obstacles should then amount to fractions of 1 eV. Thus, the clusters need not be very strong obstacles to explain the activation energy observed in macroscopic experiments at low temperatures. The present model does not explain the strong decrease of the flow stress with increasing temperature. However, as described in § 2.1, recovery plays an important role in the deformation of Al–Pd–Mn quasicrystals at high temperatures, resulting in a reduction of the flow stresses.

So far, it was assumed that the dislocations cut the clusters, certainly off-centre and not near their equators. At high temperatures, it may be easier for the dislocations to circumvent the strongly bound clusters rather than to cut them. Circumvention is a motion of the dislocations out of their glide plane which should be connected with climb. The occurrence of recovery above about 700°C shows that diffusion-controlled processes take place at most deformation temperatures. However, if the climbing process controlled the mobility of the dislocations, the activation volume should be small, i.e. of the order of magnitude of the atomic volume. This clearly contradicts the experimental results.

In quasicrystals, the dislocation motion produces a layer of phasons at low temperatures. This process is not considered in the present model. As described in § 2.3, the computer simulations by Dilger *et al.* (1997) suggest an energy for the layers of phasons of 58% of the surface energy γ. With the experimental value after Dubois (1998) of $\gamma = 17\,\mathrm{mJ\,m^{-2}}$, the generation of the phason layer would cause a friction stress of $\tau_f = 0{\cdot}58\gamma/b \cong 54\,\mathrm{MPa}$. This value corresponds to a considerable fraction of the flow stress, particularly for the deformation at high temperatures. In analogy with the production of stacking faults in crystals, the formation of the phason layer should be an athermal process, which does not influence the activation volume. If the extension of the phason layer by thermally activated jumps of individual atoms controlled the dislocation mobility, the activation volume should again be very small, in contradiction with the experimental observations. The same holds for the situation where the temperature is high enough so that the phasons diffuse away as

soon as they are created. It may therefore be concluded that the formation of phasons should not be neglected but that this is certainly not the rate controlling mechanism of dislocation motion.

In the theory of Labusch and Schwarz (1991), it is assumed that the obstacles are distributed randomly on their slip plane. Although the distribution of the Mackay-type clusters is not periodic, it is also not random. As described above, the clusters are aligned along crystallographic directions and the distances between the clusters along these directions follow a Fibonacci sequence. The random distribution assumed in the theory is certainly not a bad approximation of this non-periodic array. On the other hand, the regular character of the arrangement of the clusters is expressed in the crystallographic orientation of moving dislocations observed in the *in situ* experiments. Thus, a natural alternative description of the motion of dislocations could be a Peierls model adapted to the larger length scale in quasicrystals. Such a model does not exist up to now. Nevertheless, very simple estimates can be made by formally applying the elastic theory of the Peierls stress as described, e.g. in the textbook of Hirth and Lothe (1982). According to this theory, the Peierls energy is given by

$$U_P = \tau_P a b/\pi, \tag{8}$$

where τ_P is the Peierls stress and $a \cong 1\,\text{nm}$ is the width of the Peierls valleys. The Peierls stress should be equal to the athermal stress defined above, i.e. $\tau_P = \tau_0 = 1{\cdot}5\,\text{GPa}$. It follows that $U_P \cong 8{\cdot}7 \times 10^{-11}\,\text{N}$. This can be used to estimate the kink energy

$$\Delta G_k = (2a/\pi)(2U_P\Gamma)^{1/2}. \tag{9}$$

It turns out that $\Delta G_k \cong 1{\cdot}5\,\text{eV}$, using the above value of the line tension Γ. The activation energy of dislocation motion is then approximately equal to $2\Delta G_k$, which is slightly too large, but not in a wrong order of magnitude. However, the Peierls model in its formulation for crystals predicts an activation volume of the order of the atomic volume, i.e. it fails to describe the correct order of magnitude of the experimental activation volume. Thus, at present the cluster friction mechanism seems to be the best model to explain the dislocation mobility in quasicrystals. To establish agreement with the macroscopic deformation data, the clusters should be considered extended obstacles which are overcome in a collective way.

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