# Mechanisms of plastic deformation of icosahedral quasicrystals

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## Abstract

Icosahedral quasicrystals deform plastically by dislocation motion. The deformation behaviour can be modelled by simple equations of dislocation mobility, the damage of the quasicrystal structure and the kinetics of dislocation evolution, but fundamental questions are still discussed, like the mode of dislocation motion (glide or climb) and the role of phason defects.
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## 1. Introduction

Icosahedral quasicrystalline materials can be plastically deformed to large strains above about 70–80% of the absolute melting temperature, as first observed on polycrystals (e.g. [1]). To study the intrinsic plastic properties, single quasicrystals have been used. The drastic increase of the dislocation density during the high-temperature deformation of icosahedral Al–Pd–Mn single quasicrystals points to a dislocation mechanism of plastic deformation [2]. This view was confirmed by the direct evidence of dislocation motion during in situ deformation in a high-voltage electron microscope (HVEM) [3]. Until now, deformation induced dislocation microstructures have been observed in many icosahedral quasicrystals, but not in all of them. For example, other mechanisms have been proposed for the deformation of polycrystalline Al–Cu–Fe at ordinary strain rates [4]. The present paper discusses several aspects of the plastic deformation of icosahedral quasicrystals through the motion of dislocations. Since research is most advanced for icosahedral Al–Pd–Mn single quasicrystals, most details refer to this material.

## 2. Macroscopic deformation behaviour

At sufficiently high temperatures, iscosahedral quasicrystals can be deformed by more than 50% true plastic strain [5]. At a constant strain rate, elastic deformation is followed by a stage of a very high work-hardening rate (higher than Young's modulus), an upper and a lower yield point, a stage close to steady state deformation and finally by work-softening. The softening stage is observed,

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e.g., in Al–Cu–Fe [6] and Al–Li–Cu [7], but not in Zn–Mg–Dy [8]. In Al–Pd–Mn, the appearance of strong [5,9] or only weak softening [10,11] seems to depend on the growth conditions of the materials. It is not yet clear whether or not this softening is an intrinsic property of quasicrystals.

The steady state flow stress $\sigma$, always measured in compression, increases drastically with decreasing temperature $T$ with the absolute value of the temperature sensitivity $d\sigma/dT$ increasing, too. Below a strain rate ($\dot{\varepsilon}$) sensitive transition temperature [12] (635 °C in Al–Pd–Mn at $\dot{\varepsilon} = 10^{-5}$ s$^{-1}$), steady state deformation does not occur prior to fracture. The $T$ and $\dot{\varepsilon}$ dependencies of $\sigma$ of different icosahedral quasicrystals are quite similar, in particular if $\sigma$ is normalized by $\mu$ and $T$ by $\mu a_q^3/k$, where $a_q$ is the quasilattice constant and $k$ is Boltzmann's constant [13]. This holds for single and polygrain icosahedral quasicrystals but also for decagonal ones in different orientations and may indicate that dislocation motion during quasicrystal deformation is controlled by some very general feature like diffusion or the cluster structure. At low temperatures where steady state deformation does not occur, the specimens can nevertheless be deformed into the stage of strong work hardening [14] and under confining hydrostatic pressure [15,16]. At low temperatures, the stress where plastic deformation starts and the strain rate sensitivity $r = d\sigma/d\ln\dot{\varepsilon}$ increase only modestly with decreasing $T$.

The flow stress of quasicrystals is usually modelled in terms of three contributions, (i) the long-range elastic interactions between dislocations, treated by isotropic elasticity neglecting contributions from the phason strain field and characterized by the dislocation density $\rho$, (ii) the friction stress experienced by dislocations during their motion in the quasicrystal lattice, and (iii) a contribution from the generation of phason defects. In a macroscopic sense, the temperature and strain rate dependencies of $\sigma$ are described in the framework of thermally activated dislocation motion in crystals using an Arrhenius equation for $\dot{\varepsilon}$ (e.g. [17]). Fig. 1 shows the dependence of the activation volume $V$ on normalized stress. Different stresses correspond to different $T$ and also to different $\dot{\varepsilon}$. The data form a single curve over a
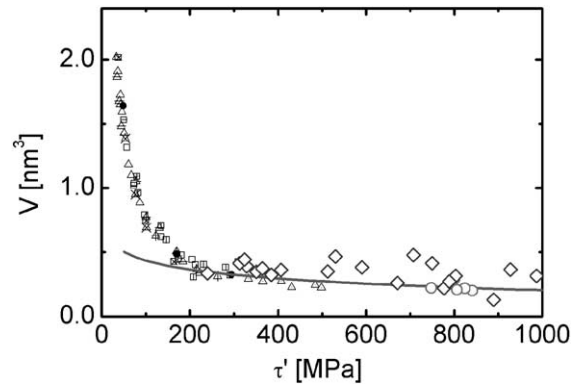


Fig. 1. Dependence of the activation volume measured by stress relaxation tests on the stress $\tau' = (\mu_o/\mu(T))m_s\sigma$; $\mu(T)$ shear modulus at temperature $T$, $\mu_o$ that at $T = 0$, $m_s$ orientation factor ($m_s \cong 0.4$). Relaxation tests were started from steady state deformation except those started from the stage of strong work hardening at low temperatures (diamonds). The highest $\tau'$ corresponds to $\sigma = 1.63$ GPa at 487 °C. After [12].

wide stress range which, with increasing stress (or decreasing temperature), first decreases rapidly and later on more gradually. Other activation parameters are discussed in [5,10,18,19].

## 3. Dislocation microstructures

In the temperature range of steady state deformation, dislocations of different Burgers vectors, which are frequently straight and crystallographically oriented, form a three-dimensional network [20,21], similar to high-temperature recovery-controlled deformation in crystals. Below that range, dislocations are concentrated in bands (Fig. 2). Considering the steep inclination of the bands against the image plane, many dislocations show bowed-out segments at low temperatures. The parallel components of the Burgers vectors are mostly perpendicular to the trace of the bands on the specimen surface, indicating that the dislocations have a large edge component and that the bands are not extending parallel to the slip plane of the dislocations. The parallel components of the Burgers vectors may be parallel or perpendicular to the compression axis. In these cases, the force exerted on the dislocations by the external stress is either a pure climb force or it is zero. Thus, though
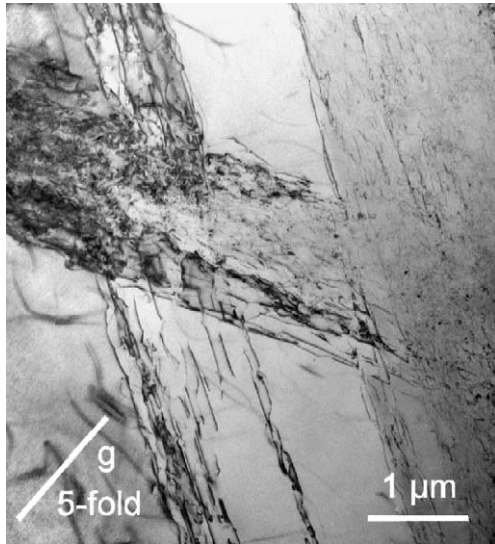
Fig. 2. Dislocation bands of deformation at 580 °C. The planes of the bands are steeply inclined against the image plane.
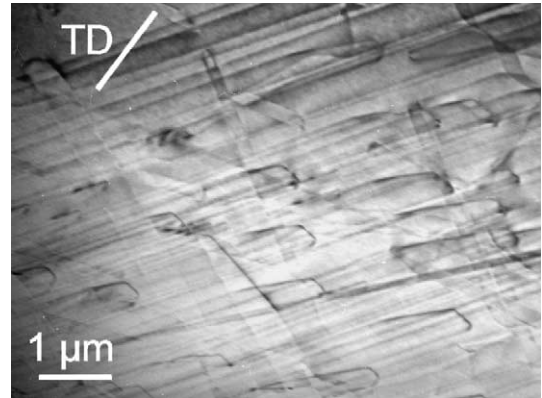


Fig. 3. Dislocations (dark lines) and traces of motion (bands of darker or brighter contrast) during an in situ straining experiment in an HVEM at about 750 °C. TD tensile direction.

the concentration of dislocations in bands at low temperatures resembles the situation in crystals, the mode of dislocation motion in quasicrystals is not clear.

## 4. Mode of dislocation motion: glide or climb?

In situ straining experiments in an HVEM show mostly straight, crystallographically oriented dislocations which move viscously and trail planar traces (Fig. 3), indicating that they move on well defined crystallographic planes [3,22]. Therefore, the plastic properties of i-Al–Pd–Mn quasicrystals have been interpreted by dislocation glide as proved for deformation at room temperature under confining hydrostatic pressure [16]. However, it was shown in Section 3 that for high temperatures this question has not been clearly answered. In order to characterize the mode of dislocation motion, it is necessary to determine independently both the plane of motion and the parallel component of the Burgers vector of the same dislocations. The planes of motion can be determined from the traces of dislocations observed during in situ straining experiments, as just described. Burgers vectors were determined by convergent beam electron diffraction of macroscopically de-

formed specimens [23] but without evidence regarding on which planes the dislocations had moved. There are several reasons to assume that climb essentially contributes to plastic deformation of i-Al–Pd–Mn. The diffusion coefficients [24] should be high enough for rapid climb in the temperature range of steady state deformation. The Burgers vectors of grown-in dislocations bordering planar faults (phason layers) and the fault vectors were found to be perpendicular to the fault planes so that these defects should have been created by climb [25]. Very recently, in situ experiments showed dislocations moving during the heating and loading phases of the tests with Burgers vectors oriented either perpendicular or inclined to the planes of motion, thus indicating climb as the main mode of dislocation motion [26].

In summary, the planar traces of moving dislocations seem not to originate from a dominance of glide, but from climb or a combination of climb and glide on preferred crystallographic planes.

## 5. Formation of phason faults

According to computer simulation studies, a layer of phason defects is trailed by the moving dislocations at low temperatures [27,28], but they diffuse away at high temperatures [29]. Phason layers extend between grown-in dislocations [25] but anneal out during in situ experiments between

660 and 690 °C (unpublished). Recently, also the annealing kinetics is studied [26]. Data scattering in the speckle contrast of diffuse X-ray scattering has shown that phason diffusion becomes important approximately in the above temperature range together with atomic diffusion [30]. Therefore, the present authors have undertaken considerable efforts to detect phason layers after deformation at lower temperatures. However, fringe contrasts at the traces of dislocations are found only in few specimens deformed at or below 610 °C (Fig. 4) and are not observed at room temperature [16]. The fringes in Fig. 4 result from phason layers, as they are bordered by a dislocation at one side, only. Since the fringes have never been observed above 610 °C, the phason defects may be assumed to diffuse away immediately in the range of steady state deformation. Nevertheless, phason strain outside the dislocation cores causes a shift of peaks in electron diffraction patterns of specimens deformed at 760 °C [31].

If phason layers are formed at low temperatures, they should yield an athermal contribution to the flow stress, similar to the generation of stacking faults in crystals. This process has been considered to make dislocations immobile and to cause
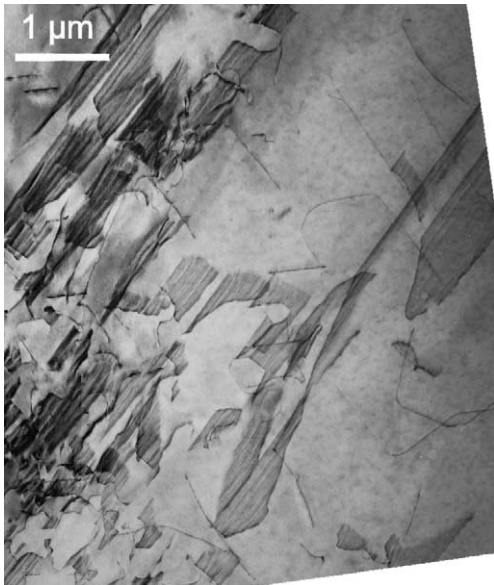


Fig. 4. Dislocations (dark lines) and planar faults (fringe contrasts) formed during deformation at 610 °C.

quasicrystals to become brittle at low temperatures. The corresponding stress contribution is estimated to only 130 MPa [32]. Thus, it would be important only at high temperatures where phason layers have not been observed. Accordingly, the role played by phason defects is not clear.

## 6. Dislocation mobility

The models for dislocation mobility were mainly established to explain the values of the activation parameters measured in macroscopic deformation tests, i.e. the activation volume $V$ of Fig. 1 and the activation (Gibbs free) energies in the order of magnitude of 2–4 eV (e.g. [19]). $V$ is an expression of the strain rate sensitivity of $\sigma$, $r = d\sigma/d\ln\dot{\varepsilon} = kT/(m_s V)$, where $m_s$ is the orientation factor. Another measure of the dependence of $\sigma$ on $\dot{\varepsilon}$ is the stress exponent $m' = d\ln\dot{\varepsilon}/d\ln\sigma = \sigma/r$. Using the data of Fig. 2 of [12], $m'$ is about 5 over the whole range of steady state deformation but increases up to 15 at lower temperatures. A quantity similar to $m'$ can be defined for the dislocation velocity $v$: $m^* = d\ln v/d\ln\sigma$ There exists a measurement on a single dislocation moving during an in situ straining experiment at changing load, yielding $m^* \cong 6$ [22]. Although the relevance of this single observation is not very high, it seems that $m^* \cong m'$.

The local stress necessary to move dislocations at a certain velocity may include a component to generate phason disorder, a component to create point defects via climb and a friction stress originating from the quasicrystal structure. For the latter contribution, two types of mechanisms are discussed, the so-called cluster friction mechanism and lattice friction mechanisms similar to the Peierls mechanism in crystals, both based on dislocation glide. The original cluster friction model [33], where strongly bound Mackay type clusters (see, e.g. [34]) are supposed strong obstacles to dislocation motion, has been refined to obtain quantitative agreement with the activation volumes (Fig. 1) [32] by considering the clusters as extended obstacles of high density that are overcome in a collective manner.

The Peierls model was originally applied to quasicrystals on an atomic scale [35], where the

dislocations form kinks with a height equal to the distances between atomic rows in the slip plane. The main objection against this model is that the kink formation energy estimated by simple elastic theory is far too low to explain the high experimental activation energies. To remove this discrepancy it may be assumed that kinks in quasicrystals form on the cluster scale [19,36,37]. The stress dependence of the activation volume following from this model is included in Fig. 1 as a solid line. It fits the experimental values at high stresses (low temperatures). The deviations at high temperatures are explained by recovery, as discussed below. Numerical estimates show that the refined cluster friction model and the Peierls model on a cluster scale predict similar macroscopic deformation data. The cluster friction model is supported by molecular dynamics simulations [38] where the dislocations move jerkily between strong spots in the quasicrystal structure, while the Peierls model fits better the straight shape of dislocations during motion and the viscous character of the latter. However, in the experiments the dislocations are straight at high temperatures but bowed out at low ones. Thus, the low-temperature Peierls mechanism cannot explain the experimental observations. Work-softening follows from both models. Deformation induced phason disorder reduces the friction stress by partially destroying the cluster structure and by facilitating kink formation [39].

A model for the dislocation mobility has to consider that the straight shape of dislocations at high temperatures has another origin than the low-temperature Peierls mechanism for glide. In many intermetallic alloys, dislocations have complex cores which extend on planes other than the glide plane, leading to a low glide mobility and to the influence of non-glide components of the stress field (e.g. [40]). In particular, the dislocations can undergo a climb dissociation (e.g. [41]), where glide is strongly impeded so that climb may become easier than glide. Double images have been observed of some dislocations moving during in situ experiments, indicating the dissociation. The core spreading is subject to geometrical constraints resulting in the straight, crystallographically oriented shape of the dislocations. The mobility should be controlled by the slowest of the processes listed above. As argued in Section 4, climb may be fast enough in the high-temperature range so that it does not control the mobility. Besides, it should lead to a stress exponent of $m^* = 1$, which is not observed. Thus, the velocity may be controlled by the friction mechanism, i.e. by the cluster structure, while the plane of motion of the dislocations and their line orientation are determined by the core spreading. To further develop these ideas, realistic atomistic calculations of the dislocation cores as well as their experimental verification are necessary. Nevertheless, dislocation motion by climb should lead (in compression) to a subsaturation of vacancies during deformation exerting a chemical force also on dislocations with zero force from the external load (Section 3) and making them climb. Such a model was proposed for the deformation of decagonal Al–Ni–Co along the periodic direction [42].

## 7. The modelling of macroscopic deformation

The macroscopic deformation parameters can be modelled by combining the characteristics of the dislocation mobility of Section 6 with the kinetics of the dislocation density $\rho$ sketched in Section 3 [43]. Usually, the dependence of the dislocation velocity on the effective stress is described by a power law. The athermal contribution to $\sigma$ due to mutual elastic dislocation interaction is taken proportional to the square root of $\rho$. The evolution of $\rho$ is characterized by a strong increase in the stage of strong work hardening, a maximum in the steady state stage and a decrease during softening. The maximum density increases strongly with decreasing temperature [44]. This can be understood by a competition between dislocation generation [22] and recovery where the steady state deformation corresponds to a balance between both [19,20]. The production of the phason defects is modelled by a stress component which decreases with increasing strain, thus taking into account the damage of the quasicrystal structure induced by the phason disorder. A model similar to the one proposed in [43] is presented in [45] refining the phason stress term by a time-dependent component considering the restoration of the intact

quasicrystal structure with time. These models describe the stress–strain curve including the yield drop effect and the softening and, in the case of [45], also the dependence of $\rho$ on strain. Another model [20] neglects the phason component and the resulting softening but considers the temperature dependence of the dislocation mobility as well as that of recovery by two different activation energies. Analytical solutions describe the dependence of the steady state $\sigma$ and $\rho$ on $T$ and $\dot{\varepsilon}$, in fair agreement with the experimental data. These simulations reveal a difficulty in analysing the data of quasicrystal deformation since the measured activation parameters, i.e. the stress exponent and the activation energies, agree neither with those of the dislocation mobility nor with those of the evolution of $\rho$. On the other hand, these data seem to be very similar for both processes. As described in Section 6, the stress exponent $m^*$ of the dislocation mobility may be about 6 and that of recovery-controlled creep, which represents mainly the dislocation evolution, is between 3 and 6 [46]. The activation energy of recovery-controlled deformation should equal that of diffusion, but diffusion may also play a role in the dislocation mobility. Since the measured activation parameters are some average of these similar data, the separation of the parameters of dislocation mobility from those of the evolution of $\rho$ is very difficult. A way out might come from measurements at low temperatures where recovery processes are less effective [14]. However, temperature change tests to measure the activation energy cannot easily be interpreted since every increment in strain is accompanied with strong hardening.

## 8. Conclusions

- If properly normalized, icosahedral quasicrystals exhibit quite similar deformation behaviour suggesting that a very general phenomenon like diffusion or overcoming the cluster structure controls the deformation.
- Although most models of dislocation mobility are based on glide, climb appears to play a dominating role.
- Little is known on the influence of the generation of phason defects on the plastic properties.

- At high temperatures, the viscous motion of straight dislocations seems to be a consequence of particular dislocation core structures.
- Steady state deformation at high temperatures may be understood by a balance between dislocation generation and recovery.

## References

[1] Shibuya T, Hashimoto T, Takeuchi S. Jpn J Appl Phys 1990;29:349.
[2] Wollgarten M, Beyss M, Urban K, Liebertz H, Köster U. Phys Rev Lett 1993;71:549.
[3] Wollgarten M, Bartsch M, Messerschmidt U, Feuerbacher M, Rosenfeld R, Beyss M, Urban K. Philos Mag Lett 1995; 71:99.
[4] Shield JE, Kramer MJ. J Mater Res 1997;12:300.
[5] Kabutoya E, Edagawa K, Tamura R, Takeuchi S, Guo JQ, Tsai A-P. Philos Mag A 2002;82:369.
[6] Giacometti E, Baluc N, Bonneville J. Philos Mag Lett 1999;79:1.
[7] Semadeni F, Baluc N, Bonneville J. In: Takeuchi S, Fujiwara T, editors. Quasicrystals. Singapore: World Scientific; 1998. p. 513.
[8] Heggen M, Feuerbacher M, Schall P, Klein H, Fisher IR, Canfield PC, Urban K. Mater Sci Eng A 2000;294–296: 781.
[9] Brunnner D, Plachke D, Carstanjen HD. Mater Sci Eng A 2000;294–296:773.
[10] Feuerbacher M, Baufeld B, Rosenfeld R, Bartsch M, Hanke G, Beyss M, et al. Philos Mag Lett 1995;71:91.
[11] Geyer B, Bartsch M, Feuerbacher M, Urban K, Messerschmidt U. Philos Mag A 2000;80:1151.
[12] Messerschmidt U, Bartsch M, Geyer B, Ledig L. In: Trebin HR, editor. Quasicrystals: structure and physical properties. Weinheim: Wiley-VCH, accepted for publication.
[13] Takeuchi S. Mater Res Soc Symp Proc 1999;553:283.
[14] Bartsch M, Geyer B, Feuerbacher M, Urban K, Messerschmidt U. Mater Sci Eng A 2000;294–296:761.
[15] Fikar J, Bonneville J, Rabier F, Baluc N, Proult A, Cordier P, et al. Mater Res Soc Symp Proc 2001;643:K7.4.1.

[16] Texier M, Proult A, Bonneville J, Rabier J, Baluc N, Cordier P. Philos Mag Lett, in press.

[17] Evans AG, Rawlings RD. Phys Status Solidi A 1969;34:9.

[18] Brunner D, Plachke D, Carstanjen HD. Mater Sci Eng A 1997;234–236:310.

[19] Messerschmidt U, Bartsch M, Geyer B, Feuerbacher M, Urban K. Philos Mag A 2000;80:1165.

[20] Messerschmidt U, Petukhov BV, Bartsch M, Dietzsch C, Geyer B, Häussler D, et al. Mater Sci Eng A 2001;319–321:107.

[21] Messerschmidt U, Ledig L, Bartsch M. Proc 8th Int Conf on Quasicrystals. J Non-Cryst Solids, accepted for publication.

[22] Messerschmidt U, Bartsch M, Geyer B, Ledig L, Feuerbacher M, Wollgarten M, et al. Mater Res Soc Symp Proc 2001;643:K6.5.1.

[23] Rosenfeld R, Feuerbacher M, Baufeld B, Bartsch M, Wollgarten M, Hanke G, et al. Philos Mag Lett 1995;72:375.

[24] Galler R, Mehrer H. Mater Sci Eng A 2000;294–296:693.

[25] Caillard D, Vanderschaeve G, Bresson L, Gratias D. Philos Mag A 2000;80:237.

[26] Mompiou F, Feuerbacher M, Caillard D. Int Symp on in situ Electron Microscopy, Nagoya, Jan 20–22, 2003. Caillard D, Feuerbacher M, private communication.

[27] Dilger C, Mikulla R, Roth J, Trebin H-R. Philos Mag A 1997;75:425.

[28] Takeuchi S, Shinoda K, Edagawa K. Philos Mag A 1999;79:317.

[29] Mikulla R, Krul F, Gumbsch P, Trebin H-R. In: Goldman AI, Sordelet DJ, Thiel PA, Dubois JM, editors. New horizons in quasicrystals: research and applications. Singapore: World Scientific; 1997. p. 200.

[30] de Boissieu M, Takakura H, Tsai AP. 8th Int Conf on Quasicrystals. Abstract.

[31] Franz V, Feuerbacher M, Wollgarten M, Urban K. Philos Mag Lett 1999;70:333.

[32] Messerschmidt U, Bartsch M, Feuerbacher M, Geyer B, Urban K. Philos Mag A 1999;79:2123.

[33] Feuerbacher M, Metzmacher C, Wollgarten M, Urban K, Baufeld B, Bartsch M, et al. Mater Sci Eng A 1997;233:103.

[34] Boudard M, de Boissieu M, Janot C, Heger G, Beeli C, Nissen H-U, et al. J Phys Condens Matter 1992;4:10149.

[35] Takeuchi S, Hashimoto T. Jpn J Appl Phys 1993;22:2063.

[36] Schall P. Diploma Thesis, RWTH Aachen, 1998.

[37] Messerschmidt U, Häussler D, Bartsch M, Geyer B, Feuerbacher M, Urban K. Mater Sci Eng A 2000;294–296:757.

[38] Schaaf GD, Mikulla R, Roth J, Trebin H-R. Mater Sci Eng A 2000;294–296:799.

[39] Takeuchi S, Tamura R, Kabutoya E, Edagawa K. Philos Mag A 2002;82:379.

[40] Bassani JL, Ito K, Vitek V. Mater Sci Eng A 2001;319–321:97.

[41] Messerschmidt U, Guder S, Häussler D, Bartsch M. Mater Res Soc Symp Proc 2001;652:Y11.6.1.

[42] Schall P. PhD Thesis. RWTH Aachen, 2002; Schall P, Feuerbacher M, Urban K. Phys Rev B, submitted for publication.

[43] Guyot P, Canova G. In: Takeuchi S, Fujiwara T, editors. Quasicrystals. Singapore: World Scientific; 1998. p. 529.

[44] Schall P, Feuerbacher M, Messerschmidt U, Urban K. Philos Mag Lett 1999;79:785.

[45] Feuerbacher M, Schall P, Estrin Y, Brechet Y. Philos Mag Lett 2001;81:473.

[46] Cannon RW, Langdon TG. J Mater Sci 1983;18:1.