

## Comment on “Cleaved surface of *i*-AlPdMn quasicrystals: Influence of the local temperature elevation at the crack tip on the fracture surface roughness”

Frohmut Rösch and Hans-Rainer Trebin

*Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany*

(Received 21 December 2007; published 16 December 2008)

Quasicrystals are intermetallic compounds with long-range quasiperiodic translational order, composed of atomic clusters, which can be interpreted as basic geometric building blocks. It is a persistent discussion whether these clusters also represent physical entities. Cleavage planes of fractured icosahedral AlPdMn as well as sputtered surfaces annealed up to about 900 K are rough with clusterlike protrusions. Fivefold surfaces annealed at higher temperatures exhibit flat terraces. Thus, obviously, the clusters cannot be termed supermolecules. However, experiments and numerical simulations indicate that fracture is influenced by the clusters. Thus, they determine physical properties. In a recent paper, Ponson *et al.* [Phys. Rev. B **74**, 184205 (2006)] investigated experimental fracture surfaces of AlPdMn and questioned the signature of the clusters. In this comment, we study the self-affinity of cleavage planes obtained by molecular-dynamics simulations. We conclude that the findings of Ponson *et al.* are *not* excluding a physical role of the clusters in quasicrystals.

DOI: [10.1103/PhysRevB.78.216201](https://doi.org/10.1103/PhysRevB.78.216201)

PACS number(s): 62.20.M-, 64.60.Ht, 68.35.Ct, 81.40.Np

One method to analyze the roughness of fracture surfaces is to calculate the height-height correlation functions. These reveal scaling properties (see Ref. 1 for a review paper) with a “universal” roughness exponent of about 0.8 for a wide range of materials. However, up to now, no theoretical model is able to satisfactorily capture this self-affinity. Thus, it is hard to interpret microscopic properties of the investigated structures starting from the scaling behavior. It might even not be possible to distinguish a fractured from a sputtered surface, as the roughness exponents of both surfaces can lie in the same range.<sup>2,3</sup> Although the scaling behavior of fracture surfaces seems to be universal, the range of length scales in which it is valid may strongly vary for different materials. It has been argued that the corresponding cut-off length  $\xi$  is related to the size of the process zone  $R_c$ .<sup>4</sup> Inside this region, linear elastic predictions do not fit the real deformation field. Such a nonlinear and dissipative zone always exists, as atomic bonds break at the crack tip. The behavior on and below this scale determines whether, how, and where a crack travels.  $R_c$  should therefore be related to the microstructure. In the following, we investigate the role and interpretation of  $\xi$  for fracture surfaces of icosahedral quasicrystals.

The roughness of *i*-AlPdMn fracture surfaces was analyzed in a recent paper by Ponson *et al.*<sup>5</sup> They found scaling properties which resemble those of various disordered materials. The height-height correlation function reveals a self-affine behavior from the atomic scale up to  $\xi \approx 2$  nm. The corresponding Hurst exponent  $H$  is found to be about 0.72 (see Fig. 2 of Ref. 5). The authors pointed out that the self-affine region includes the radius of the clusters  $r_c \approx 0.5$  nm, which are inherent in the structure. It is stated that the morphology of the fracture surfaces therefore does not reflect the cluster distribution. Thus, the influence of the clusters on physical properties of *i*-AlPdMn is questioned. A damage mechanism involving dislocations is then motivated from molecular-dynamics simulations of two-dimensional (2D) model quasicrystals.<sup>6</sup> The local temperature rise at the crack tip is made responsible for a suggested nanoplastic behavior within the process zone.

First, we counter that the influence of the clusters on fracture surfaces has been pointed out in previous experimental findings<sup>7,8</sup> and computer simulations.<sup>6,9,10</sup> Second, we shortly comment on the proposed mechanism within the process zone. Dislocation assisted fracture is indeed observed in molecular-dynamics simulations of two-dimensional quasicrystals.<sup>6</sup> In three dimensions, this would correspond to quasicrystals which are quasiperiodic within a plane and periodic in the third direction, e.g., decagonal quasicrystals. A straight dislocation line can be realized in these structures. In simulations of three-dimensional icosahedral quasicrystals, however, it is very hard to create and drive dislocations.<sup>11</sup> Perfect brittle fracture without dislocation activity is observed in numerical experiments.<sup>9</sup> Thus, the suggested nanoplastic behavior seems unlikely in *i*-AlPdMn. Plastic deformation in the brittle domain has only been reported for compression or shear deformation under confining pressure.<sup>12</sup> The dislocations seem to move by climb. No evidence of dislocation activity is detected in areas where fracture occurs. The suggested local temperature rise at the crack tip is supported by simulations [see, e.g., Fig. 3 and movie (Ref. 35) of Ref. 9]. But the definition of a temperature in a nonequilibrium system poses problems. The value strongly depends on the region over which an average is taken. Obviously, atoms at a breaking bond move fast and thus have a high kinetic energy. So, even temperatures up to the magnitude of the melting temperature might be defined.

Third, we show that it is hard to reason properties of the microstructure from the self-affine behavior of fracture surfaces. For this purpose, experimental findings at room temperature are compared to results from atomistic simulations. The surface data of AlPdMn used by Ponson *et al.*<sup>5</sup> was obtained by scanning tunneling microscopy (see Refs. 7 and 8). The molecular-dynamics simulations have been performed in a representative icosahedral model quasicrystal at low temperature and load.<sup>9,10</sup> The height of the fracture surfaces is derived by geometrical scanning.<sup>9</sup> The length scale in the simulations is given by  $r_0$ , the shortest distance between two atoms in the model quasicrystal. The icosahedral

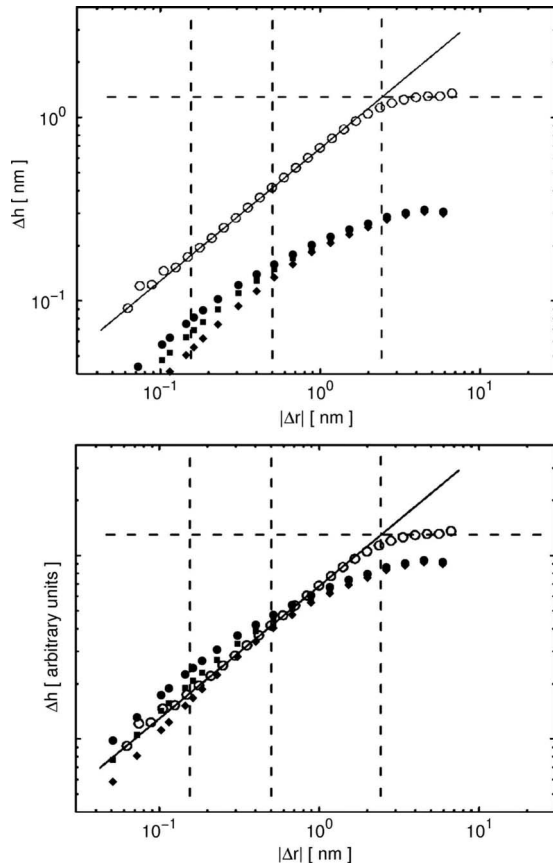


FIG. 1. Height-height correlation function  $\Delta h$ . Open symbols: experiment; solid symbols: simulations [the radius  $r$  of the scanning sphere is varied: the size of an atom (disks),  $r=r_0$  (squares), and  $r=2r_0$  (diamonds) are used]. Vertical lines indicate the atomic radius, the cluster radius, and  $\xi$ . The simulated results (top) are scaled (bottom) to allow a direct comparison of the characteristics of the curves. For details, see text.

system, the temperature as well as the contrast of the scanning images differ from the experimental situation. In contrast to the experimental data, no anisotropy due to imaging and no noise is present in the simulated images. The analysis of experimental self-affine surfaces further may suffer from, e.g., misorientation, signal amplification, and local geometric filtering.<sup>13</sup> In spite of the difficulties in data acquisition and processing, qualitative aspects of the experiments are resembled well by the simulations.<sup>9</sup> In Fig. 1 (top) experimental findings (open symbols; see Fig. 2 of Ref. 5) are compared to simulated results [solid symbols (see Rösch *et al.*<sup>9</sup>): orientation 2<sub>2</sub>, load  $k=1.3$ ]. Obviously, the data sets differ due to, e.g., the different scanning techniques, temperatures, and models. To allow a direct comparison the height-height correlation function derived from the simulations  $\Delta h_{\text{sim}}$  is scaled by a factor of 3 (see Fig. 1, bottom). This necessary shift, e.g., indirectly shows that the experimental surface has a higher root-mean-square roughness than the one simulated at very controlled conditions at low temperature. However, the absolute values of  $\Delta h$  are not relevant for the following considerations; as we concentrate on  $\xi$  and the characteristics of the curves to answer the question whether  $\Delta h$  can give valuable information on the role of the clusters. For a crack

front propagating between indestructible spherical clusters, one, e.g., could expect a drastic change in the behavior of  $\Delta h$  for  $\Delta r \approx r_c$ , where  $r_c \approx 0.5$  nm is the radius of the clusters. It is evident from Fig. 1 that neither for the experiment nor for the simulations a hard crossover can be observed. However,  $\Delta h_{\text{sim}}$  obviously seems to be a bit more curved.<sup>14</sup> To investigate how the scanning conditions influence  $\Delta h$ , we vary the radius  $r$  of the scanning sphere. The size of an atom (disks in Fig. 1),  $r=r_0$  (squares in Fig. 1), and  $r=2r_0$  (diamonds in Fig. 1) are used. Obviously, the form of the curves depends on the tip size. If the size of the tip and the size of the structure become comparable, an interpretation of the curves is difficult. All curves give  $H \approx 0.7$  for the first few points on the left in Fig. 1. For the simulations  $\xi \approx 1$  nm may be assumed. Thus, as in the experimental findings, the self-affine behavior can include the radius of the clusters  $r_c$ . For the computer simulations, detailed analyses prove that the clusters influence fracture behavior.<sup>9</sup> This contrasts with the interpretation of Ponson *et al.*<sup>5</sup> They concluded from  $\xi > r_c$  that the clusters cannot be responsible for the morphology of the fracture surfaces. Our simulations show the opposite: the clusters play a crucial role despite  $\xi \geq r_c$ . Furthermore, there is no evident deviation from a linear behavior in  $\Delta h_{\text{sim}}$  in the region pointed out by Ponson *et al.*<sup>5</sup> Thus, the simulations additionally show that the length scale of the clusters does not need to have an *obvious* influence on the height-height correlation function despite their relevance in fracture behavior. This is understandable from the fact that the clusters are not unbreakable supermolecules giving a smallest scale by their diameter. So, there is not a single relevant length scale and the lower limit of the power-law behavior is determined by the atomic size rather than by the radius of the clusters. In experiments, details of the height-height correlation function may further be hidden by limitations in the resolution of the scanning devices and any additional noise.

Fourth, we demonstrate that the relation  $R_c \geq r_c$  can be seen as a consequence of the deformation behavior of the clusters. An icosahedral quasicrystal macroscopically behaves elastically isotropic. Locally, this behavior can change due to the clusters and the glue atoms in between. So, if the clusters should influence physical properties, their local deformation close to the crack tip should deviate from the linear elastic prediction. Such a deviation, however, only is possible *within* the process zone. Thus, the size of the process zone naturally can include the cluster scale. So, it is easy to argue in favor of a physical role of the clusters in quasicrystals from  $\xi \geq r_c$ . From this point of view an extended process zone size is easily explainable without the assumption of an additional dislocation assisted process.

Overall, it is difficult to deduce the role of the microstructure from the scaling properties of fracture surfaces. From our discussion it is now evident that the results of Ponson *et al.*<sup>5</sup> are no good for vitiating the role of clusters in the fracture process.

Support from the Deutsche Forschungsgemeinschaft under Contract No. TR 154/25-1 and by the European Network of Excellence on Complex Metallic Alloys (Contract No. NMP3-CT-2005-500140) are gratefully acknowledged.

- <sup>1</sup>E. Bouchaud, *J. Phys.: Condens. Matter* **9**, 4319 (1997).
- <sup>2</sup>Z. Csahok, Z. Farkas, M. Menyhard, G. Gergely, and Cs. S. Daroczi, *Surf. Sci.* **364**, L600 (1996).
- <sup>3</sup>T. Lindström, J. Isidorsson, and G. A. Niklasson, *Thin Solid Films* **401**, 165 (2001).
- <sup>4</sup>D. Bonamy, L. Ponson, S. Prades, E. Bouchaud, and C. Guillot, *Phys. Rev. Lett.* **97**, 135504 (2006).
- <sup>5</sup>L. Ponson, D. Bonamy, and L. Barbier, *Phys. Rev. B* **74**, 184205 (2006).
- <sup>6</sup>R. Mikulla, J. Stadler, F. Krul, H.-R. Trebin, and P. Gumbsch, *Phys. Rev. Lett.* **81**, 3163 (1998).
- <sup>7</sup>Ph. Ebert, M. Feuerbacher, N. Tamura, M. Wollgarten, and K. Urban, *Phys. Rev. Lett.* **77**, 3827 (1996).
- <sup>8</sup>Ph. Ebert, F. Yue, and K. Urban, *Phys. Rev. B* **57**, 2821 (1998).
- <sup>9</sup>F. Rösch, Ch. Rudhart, J. Roth, H.-R. Trebin, and P. Gumbsch, *Phys. Rev. B* **72**, 014128 (2005).
- <sup>10</sup>F. Rösch, H.-R. Trebin, and P. Gumbsch, *Philos. Mag.* **86**, 1015 (2006).
- <sup>11</sup>G. D. Schaaf, J. Roth, and H.-R. Trebin, *Philos. Mag.* **83**, 2449 (2003).
- <sup>12</sup>M. Texier, A. Joulain, J. Bonneville, L. Thilly, and J. Rabier, *Philos. Mag.* **87**, 1497 (2007).
- <sup>13</sup>J. Schmittbuhl, J.-P. Vilotte, and S. Roux, *Phys. Rev. E* **51**, 131 (1995).
- <sup>14</sup>One has to note here that the model system does not fully capture the self-similarity rules of icosahedral quasicrystals.