

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

L. Barbier, D. Bonamy, and L. Ponson^{*,†}

IRAMIS, SPCSI, Group Complex Systems and Fracture, CEA, F-91191 Gif sur Yvette, France

(Received 10 September 2008; published 16 December 2008)

In their Comment on our recent paper [Ponson *et al.*, Phys. Rev. B **74**, 184205 (2006)], Rösch and Trebin reinterpret our experimental findings on cleavage surfaces of *i*-AlPdMn quasicrystals (QC) using molecular-dynamics simulations of crack propagation in icosahedral model QC. Here, we detail and maintain our initial interpretation of the roughness of QC fracture surfaces in terms of damage mechanisms and temperature elevation in the vicinity of the crack tip. We then discuss the outputs of their numerical simulations and show that the numerical surfaces display different properties than the experimental ones, making the use of the features pointed out by the simulations difficult in interpreting the experimental data. Thus, we maintain the main conclusion of our paper that the existence of clusters in the QC structure cannot be evidenced from the cleavage experiment of Ebert and coworkers [Phys. Rev. Lett. **77**, 3827 (1996); Phys. Rev. B **57**, 2821 (1998)].

DOI: 10.1103/PhysRevB.78.216202

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

Comparison between experimental data and result of simulations is always of great interest in catching the main features and detailing individual processes of dynamic systems. Such an extended discussion was indeed missing in our recent paper¹ where an analysis of the data obtained by Ebert and co-workers^{2,3} on quasicrystal (QC) cleavage surfaces is reported. Only numerical results on two-dimensional (2D) decagonal model QC were mentioned⁴ to support the idea that a process zone may exist in quasicrystals. An extended discussion must involve the more recent papers of Rösch and co-workers^{5,6} where results of molecular dynamic simulations on three-dimensional (3D) binary QC with icosahedral symmetry were presented.

The problem under discussion is to decide whether fracture surfaces may reveal the role of clusters of atoms entering in the QC structure as physical entities. This was claimed by Ebert and co-workers^{2,3} from a qualitative first analysis of their experimental surfaces and from computer simulations.^{5,6} In our statistical analysis of the very same experimental data, we conclude that the cluster size $r_c = 0.5$ nm does not appear as a characteristic length scale on the QC fracture surfaces. This is mainly shown by computing the height-height correlation function $\Delta h(\Delta \vec{r}) = \langle [h(\vec{r}_0 + \Delta \vec{r}) - h(\vec{r}_0)]^2 \rangle_{r_0}^{1/2}$ that exhibits a power-law behavior with exponent $\zeta \approx 0.75$ from the atomic size up to ≈ 2 nm. This means that there is *no relevant length scale* within this range. Such a behavior has been observed for a great variety of materials such as silica glass, metallic alloys, or mortar,⁷ suggesting that this scaling is universal. More recently, it was shown that the upper limit of this scaling regime is set by the process zone size R_c .^{8–10} At larger length scales, another roughness regime is observed that is characterized by a smaller exponent or logarithmic correlations of height fluctuations. This second regime is fully understood using linear elastic fracture mechanics extended to heterogeneous media^{9–11} and is reminiscent of a brittle failure.

In their Comment,¹² Rösch and Trebin claim that the observed scaling behavior of QC fracture surfaces is compatible with a crack propagation between the clusters, and so,

this observation is not in contradiction with a physical role of the clusters during failure processes. At first, the damage mechanisms—nucleation and behavior of dislocations—suggested by the scaling behavior of QC surfaces is discussed. We agree that the sentence in Ref. 1 “This process zone would result from effective dislocation creation and motion as in monocrystals.” may be confusing and should not be taken into account too literally. In elastic materials, all the mechanical energy released upon crack growth is dissipated in a small zone around the crack tip—the so-called process zone—where all the damage occurs. Depending on the material, this damage can take various forms: nucleation of microcracks for brittle materials (mortar, wood, rocks, etc.) or damage cavities for ductile materials (metallic alloys). It was shown however that below the size of the process zone and independently of the precise nature of damage spreading, the fracture surfaces exhibit *universal* scaling properties characterized by a peculiar shape of the correlation function—Family-Vicsek scaling given by Eq. (4) of Ref. 1—and a scaling exponent $\zeta \approx 0.75$, both observed on QC fracture surfaces. These damage processes suggested by the morphology of QC fracture surfaces have been also directly observed on 3D simulations.

Temperature definition is next questioned. We agree that it is not easy to define rigorously a local temperature field (and stress or displacement fields as well). However, there is no doubt that—because of irreversible dissipative processes—the temperature increases within the process zone as experimentally observed.¹³ Outside of a zone with size R_T of the same order as R_c , the temperature decays as $1/r$, r referring to the distance from the crack tip.¹⁴ In addition, the temperature value extrapolated from Eq. (7) in Ref. 1 makes our interpretation consistent in a more quantitative way. On the theoretical side, molecular-dynamics simulations^{5,6} first show that sound waves are emitted from the crack tip.¹⁵ In addition, a movie of the cleavage process was produced showing that bonds are not only broken at the crack tip but also away of it.¹⁵ Both movies illustrate qualitatively the two main ingredients of the scenario we propose: existence of an

extended process zone around the crack tip and local temperature elevation.

Following our approach, comparison with experimental data is done through computation of the correlation function $\Delta h(\Delta \vec{r})$. Since height and distance scales are fixed by the *i*-AlPdMn QC structure, it is mentioned that Δh is lower by a factor of 3 than the experimental data. Smoothing or experimental noise would modify only the fluctuation level at short scale, this adding a constant term to $\Delta h(\Delta \vec{r})$. This constant becomes negligible compared to the roughness level at large scale. In other words, short-range effects such as finite size of the probe tip cannot be taken into account by a vertical shift of the whole log-log plot, i.e., a multiplication by a factor of 3. This suggests that the failure mechanisms at the origin of the experimental fracture surfaces and those involved in the simulations might be different. This is confirmed by a careful comparison of the correlation functions $\Delta h(\Delta \vec{r})$ computed on numerical and experimental fracture surfaces. It is often very useful to represent its logarithmic derivative $\frac{\partial \ln(\Delta h)}{\partial \ln(\Delta z)}$ so that a true power-law variation $\Delta h \sim \Delta r^\zeta$ appears as a plateau regime. This quantity is plotted on Fig. 1 where the simulation results are the data of Rösch and Trebin¹² as given in their comment. For the experimental surface, a plateau regime with $\zeta \approx 0.72$ is well observed from the atomic size up to a cutoff length scale $\xi \approx 1.5$ nm consistent with the power-law variation in the correlation function on this range of length scales as reported in Ref. 1. However, it appears clearly now in this representation that the correlation function derived from the surface obtained by simulations do not follow a power-law behavior, whatever the radius of the scanning sphere is. The geometry of the numerical surface is investigated in more detail in the inset of Fig. 1 where its correlation function is represented in a semilogarithmic representation. The linear variation observed from $\Delta r \approx 0.3$ nm up to the image size suggests logarithmic correlations of the surface height. This observation is in perfect agreement with the scenario of a brittle failure with limited damage processes where the crack front would propagate between the basic microstructural features of the system—the clusters of size $r_c \approx 0.5$ nm—and proposed by Rösch and co-workers.^{5,6} As a result, the differences of roughness amplitude and correlation function behavior strongly suggest that the mechanisms responsible for the self-affine roughness observed experimentally are not captured in the simulation.

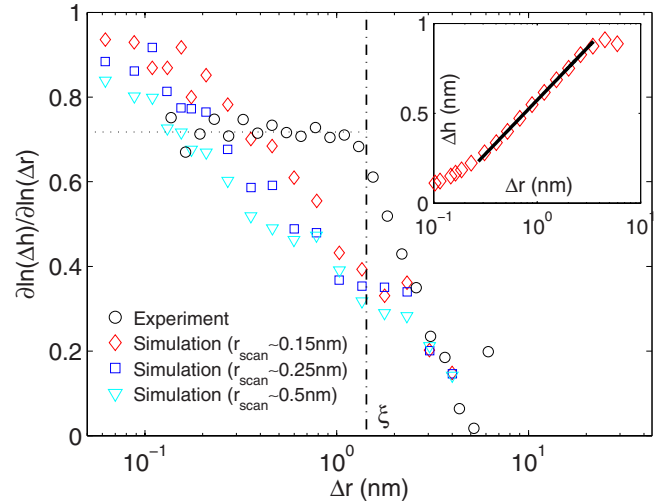


FIG. 1. (Color online) Logarithmic derivative of the correlation function of experimental and numerical fracture surfaces. In this representation, a true power-law behavior appears as a plateau. The inset shows the correlation function obtained from the simulations in a semilogarithmic representation.

In conclusion, the experimental observation of a height correlation function $\Delta h(\Delta \vec{r})$ with a self-affine universal behavior is the indication that no scale is relevant in the system between the atomic scale and R_c . This further allows concluding that the influence of clusters on the surface roughness, if such clusters (Bergman or MacKay) exist as physical entities, is hidden by the damage occurring within the process zone. Comparison with simulations is challenging but the level of the surface roughness and its scaling properties, rather different than in the experiments, make difficult the use of the features pointed out by the simulation in interpreting the experimental data. Thus, we maintain the main conclusion of our paper that the existence of clusters in the QC structure cannot be evidenced from the cleavage experiment of Ebert and co-workers.^{2,3} Thanks to the comment, it is finally suggested that a fracture experiment at low temperature and ultralow velocity might allow to make the process zone smaller, allowing a possible comparison with simulations.

*Present address: Division of Engineering and Applied Science, California Institute of Technology, Pasadena, California 91125, USA.

†ponson@caltech.edu

¹L. Ponson, D. Bonamy, and L. Barbier, Phys. Rev. B **74**, 184205 (2006).

²P. Ebert, M. Feuerbacher, N. Tamura, M. Wollgarten, and K. Urban, Phys. Rev. Lett. **77**, 3827 (1996).

³P. Ebert, F. Yue, and K. Urban, Phys. Rev. B **57**, 2821 (1998).

⁴R. Mikulla, J. Stadler, F. Krul, H.-R. Trebin, and P. Gumbsch, Phys. Rev. Lett. **81**, 3163 (1998).

⁵F. Rösch, C. Rudhart, J. Roth, H.-R. Trebin, and P. Gumbsch, Phys. Rev. B **72**, 014128 (2005).

⁶F. Rösch, H.-R. Trebin, and P. Gumbsch, Philos. Mag. **86**, 1015 (2006).

⁷L. Ponson, D. Bonamy, and E. Bouchaud, Phys. Rev. Lett. **96**, 035506 (2006).

⁸S. Morel, D. Bonamy, L. Ponson, and E. Bouchaud, Phys. Rev. E **78**, 016112 (2008).

⁹L. Ponson, Ann. Phys. **32**, 1 (2007).

¹⁰D. Bonamy, L. Ponson, S. Prades, E. Bouchaud, and C. Guillot, Phys. Rev. Lett. **97**, 135504 (2006).

- ¹¹S. Ramanathan, D. Ertas, and D. S. Fisher, *Phys. Rev. Lett.* **79**, 873 (1997).
- ¹²F. Rösch and H.-R. Trebin, Comment, *Phys. Rev. B* **78**, 216201 (2008).
- ¹³P. R. Guduru, A. T. Zehnder, A. J. Rosakis, and G. Ravichandran, *Eng. Fract. Mech.* **68**, 1535 (2001).
- ¹⁴J. R. Rice and N. Levy, *The Physics of Strength and Plasticity* (MIT Press, Cambridge, 1969), p. 277.
- ¹⁵Electronic auxiliary material accompanying Ref. 5.