Response to "Comment on 'Nanoindentation hardness anisotropy of alumina crystal: a molecular-dynamics study'" [Appl. Phys. Lett. 94, 146101 (2009)]

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Tymiak *et al.*[1] raised important issues regarding nanoindentation in the light of experiments and continuum calculations at larger length scales than in our molecular dynamics (MD) simulations.[2] As pointed out by Tymiak *et al.*,[1] indenter geometry, especially its precise control to delineate crystallographic orientations of the substrate, is essential if the nanoindentation hardness anisotropy found in our MD simulations[2] is to be observed experimentally. To show the effect of indenter geometry, Fig. 1 compares MD simulation results on the von Mises (or equivalent tensile) stress distribution[3] under a Berkovich indenter[1] at indentation depth $h=1.5$ Å on (0001) α-alumina surface with (a) an atomically sharp indenter tip and (b) a round tip with radius 300 Å. The figure illustrates a marked difference in stress distribution below the indenter: The stress concentrates, thereby causing the breaking of atomic bonds, just beneath the atomically sharp indenter in (c), while the stress concentration and associated plastic activities occur away from the tip center under the round indenter (which is similar to previous MD simulation results for Cu)[3] in (d). Such difference in stress distribution results in widely different load-displacement relations, as was observed in our nanoindentation simulations on silicon carbide crystal with pyramidal-shape[4] and flat-punch[5,6] indenters. Also, it should be noted that highly nonlinear repulsive interatomic potentials and atomic discreteness play an important role in determining indenter-substrate interaction at small $h(<5$ Å), for which interpretation based on linear elasticity and continuum mechanics may not apply. For example, though the estimated hardness value reaches ~500 GPa at $h=2$ Å as pointed out by Tymiak *et al.*,[1] the maximal pressure remains an order of magnitude smaller (less than 60 GPa). As such, we agree with the comment by Tymiak *et al.*[1] that the hardness size effect for $h<15$ Å in our paper is distinct from those observed experimentally at much larger length scales ($h>500$ Å).[7–9] Regarding the estimation of hardness values, we thank Tymiak *et al.*[1] for pointing out the underestimation in our paper[1] due to the use of total indentation depth h_t instead of the contact indentation depth h_c. We have recalculated the hardness values using h_c (indenter and substrate surfaces are regarded in contact if their distance is within 6 Å) to obtain 56% larger hardness value for $h_t=19.5$ Å for (0001) indent. This, however, does not affect any conclusions regarding hardness anisotropy.

Another important point raised by Tymiak *et al.*[1] is the validity of the interatomic potential[10] used in our MD simulation.[2] Though fundamental understanding of the structure and dynamics of lattice defects in alumina is a highly complex problem[11] and is beyond the scope of our paper,[2] we have performed a simple test by calculating the ideal shear strength[12] of the basal plane as the maximum gradient of the generalized stacking fault energy along the minimum-energy path with MD (Ref. 13) as well as quantum-mechanical (QM) calculation based on the density functional theory (DFT) using plane-wave basis sets, generalized gradient approximation for the exchange-correlation energy, and ultrasoft pseudopotentials to describe the interaction between valence electrons and ions.[14] The MD result, 16.3 GPa, agrees well with the *ab initio* QM result, 18.9 GPa, showing the adequacy of our interatomic potential[10] to describe such slip processes. Though the few initially activated defects in our indentation simulations are dislocations at small indent depth ($h<20$ Å),[2] more extensive plastic deformations, such as in our impact damage simulations,[13] do involve twins, which play an important role in plastic deformations

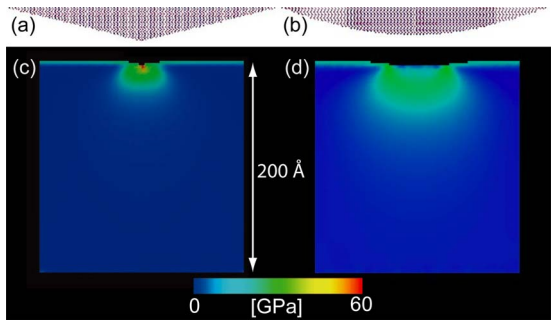

FIG. 1. (Color online) Berkovich indenter with (a) an atomically sharp indenter tip and (b) a round indenter tip with radius 300 Å. Molecular dynamics simulation results on von Mises stress distribution under a Berkovich indenter at indentation depth $h=1.5$ Å on (0001) α-alumina surface with (c) the atomically sharp indenter tip and (d) the round indenter tip.

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in alumina as pointed out by Tymiak *et al.* Our MD simulation of impact damage on alumina also shows a phase transformation,[13] which deserves further QM study to be compared with experimentally observed contact-induced phase transformation.[15,16]

In summary, our MD simulation of nanoindentation anisotropy of alumina crystal has been validated by first-principles DFT calculations where possible, and its findings are likely valid at nanometer indentation depths. However, their generalization to larger indentation depths and different indenter shapes is nontrivial and would require further study.

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