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Nanindentation of NiAl and Ni$_3$Al crystals on (100), (110), and (111) surfaces: A molecular dynamics study

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Molecular dynamics simulations were performed to study the nanindentation of NiAl and Ni$_3$Al crystals on three surfaces: (100), (110), and (111). The calculated load-displacement curves show discrete drops at certain indentation depths, indicating dislocation bursts during indentation. The hardness values for the two materials were found to depend significantly on the indented crystallographic plane: the (100) surface is the softest for NiAl and the hardest for Ni$_3$Al. We also found distinctive deformation activities in the subsurface region in Ni$_3$Al crystals, while dislocation loops propagate deep into the substrate in NiAl systems. © 2014 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [http://dx.doi.org/10.1063/1.4867168]

Nickel aluminide is an intermetallic compound with important technological applications because of its light weight as well as its resistance to oxidation, corrosion, structural deformation, and yield strength at high temperatures. In intermetallic compounds, the coexistence of metallic and covalent interatomic bonding makes their mechanical properties highly nontrivial. An example is the anomalous yield strength of Ni$_3$Al at elevated temperatures. Unlike ordinary materials, it exhibits maximum strength before melting, as the temperature increases. The strength of nickel aluminide also depends on crystallographic orientations. In transition metal alloys such as NiAl, structural transformation is observed under applied stress. In the molecular dynamics (MD) simulation of nanowires carried out by Park, the strain response of NiAl was shown to change from brittle to super elastic via martensitic phase transformation. Zhang et al. suggested that in NiAl, dislocations can serve plastic accommodation during the growth of martensitic transformation. Using transmission electron microscopy, Zhu et al. studied the orientation dependence of creep behavior in Ni$_3$Al single crystal and observed a crossover of slip systems—from octahedral to cubic planes—between the primary and secondary creep stages. Kozlov et al. studied the anomalous temperature dependence of the yield point in Ni$_3$Al and attributed it to the anisotropic atomic arrangement in dislocation glide planes. Though nickel aluminide compounds have been widely used in gas turbines and jet engines, their brittleness hinders their use as thin films in many engineering applications. One approach toward overcoming this difficulty may be through nanostructural design. In fact, unique mechanical properties have been observed experimentally for Ni$_3$Al nanocubes and through MD simulations for Ni$_3$Al nanowires. A key to controlling these nanomechanical properties is the atomistic understanding of anisotropic mechanical responses on different crystallographic surfaces.

Nanoindentation is a widely used experimental technique to examine the mechanical response of materials, including the slip system, through localized damage induced by a sharp indenter tip. A number of nano-to-micro indentation studies has been carried out on NiAl and Ni$_3$Al single crystals, multilayered thin films, NiAl-coated Ni substrate, and other Ni alloys, which shows an indentation size effect and anisotropic hardness with respect to the indenter orientation. MD simulations have been used to investigate atomistic processes during nanoindentation for metals and ceramics. Although extensive research has been done on nickel aluminide systems, a comprehensive study of their mechanical responses is still lacking. In this work, we have performed nanoindentation MD simulations on three nickel aluminide surfaces: (100), (110), and (111) for B2-NiAl and L1$_2$-Ni$_3$Al crystals.

Figures 1(a)–1(c) show the unit cell structure of B2 NiAl and L1$_2$ Ni$_3$Al crystals and a schematic of a nanoindentation simulations setup. We used an embedded atom method (EAM) type potential developed by Chen, Srolovitz, and Voter to investigate the NiAl and Ni$_3$Al systems. With EAM’s interatomic potential, Chen et al. studied the grain boundary (GB) structure, GB cohesive energy, and stain distribution around GBs. To perform MD simulations of NiAl systems, we also examined the cohesive energy, bulk modulus, and surface energy of B2-NiAl, which show reasonable agreement with the literature. The film dimensions for the six systems are approximately 180 Å, 180 Å, and 170 Å in the x-, y-, and z- directions, respectively. NiAl systems with the (100), (110), and (111) surfaces contain 450,560, 560,000, and 476,928 atoms. The numbers of atoms for Ni$_3$Al crystals with the (100), (110), and (111) surfaces are 486,720, 492,544, and 471,744, respectively. Periodic boundary conditions are applied in the x- and y- directions perpendicular to the indentation direction. The thin film is initially quenched to 0 K to relax the surfaces and is gradually heated up and thermalized at 300 K. A thin layer of atoms, 5 Å from the bottom of the film in the z- direction, is fixed to hold the film during simulation. In all simulations, we use a
four-faced pyramidal-shape rigid indenter with a 90° edge angle cut out of an fcc crystal. The indenter atoms interact with film atoms through pure repulsion. One MD time step is 2.5 fs throughout the simulations. During the loading phase, the indenter is moved into the film by 0.5 Å for 1000 time steps. Subsequently, we relax the system by holding the indenter for 9000 time steps. We repeat this process until the total indentation depth reaches approximately one-quarter of the film thickness, corresponding to 40 Å from top surface. During unloading phase, we use the same schedule except for reversing the direction of the indenter displacement. To identify defect atoms, we used coordination number and common neighborhood parameter (CNP).

Table I summarizes hardness values (i.e., the indenter load divided by the projected indentation area) obtained for the six simulations. In the NiAl systems, the (100) surface is notably softer than the (110) and (111) surfaces. On the other hand, the (100) surface is harder than the other two surfaces in the Ni₃Al systems.

Figure 2 shows the load-displacement curves ($P-h$) and hardness for the NiAl (100) and Ni₃Al (100) systems. We observe several drops in the $P-h$ curves during the loading phase (pop in) indicating discrete deformation events in our systems. The hardness values of the six systems exhibit the indentation size effect and crystallographic-orientation dependency.

Figure 3 below shows snapshots of the dislocation activities in NiAl (100) at the indentation depth $h = 40$ Å. During indentation, dislocations form a loop structure (pointed by the yellow arrow), which glides in the $\langle 100 \rangle$ direction moving away from the indenter. The loop develops into a skewed square shape with the sides oriented towards the $\langle 112 \rangle$ and $\langle 112 \rangle$ directions (see Fig. 3(b)). At $h = 40$ Å, we also observe the nucleation of second dislocation loop (pointed by the red arrow).

Figure 4 shows the dislocation loop under the indenter with half of the top surface of the system cut away on the (011) plane. In the NiAl (110) and NiAl (111) simulations, two dislocation loops are formed one after the other, parallel to each other and separated by about 15 Å. In contrast to the NiAl systems, dislocation activities are rather confined within the subsurface regions in the Ni₃Al crystals.

### Table I. Hardness of NiAl and Ni₃Al with the (100), (110), and (111) surfaces.

|           | (100) | (110) | (111) |
|-----------|-------|-------|-------|
| NiAl      | 11.9  | 16.9  | 17.0  |
| Ni₃Al     | 21.5  | 17.8  | 18.4  |

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dislocation activities near the indenter at the indentation depth $h = 25 \text{Å}$. By increasing indentation depth, dislocations nucleate from the corner of the indenter and develop into a V-shape that subsequently travels away from the indenter via edge dislocations on the \{111\} family of planes. Figure 5(b) shows the distribution of surface atoms in the vicinity of the V-shape slip planes looking down on the (100) plane. Burgers vector analysis shows that the two partial dislocations, $\frac{1}{3}(112)$ and $\frac{1}{2}(121)$, comprise the V-shape dislocations. This partial dislocation accounts for the 1.1 Å height difference of the atoms within the V-shape region compared to outside.

In summary, we performed MD simulations of nanoindentation on NiAl and Ni$_3$Al crystals with the (100), (110), and (111) surfaces. Discrete drops in the obtained $P-h$ curves were found to arise from dislocation bursts underneath the indenter. The hardness of the NiAl and Ni$_3$Al system shows significant dependence on the crystallographic planes, specifically the lowest hardness for NiAl (100) and the greatest value for Ni$_3$Al (100). Our MD simulations have revealed that plastic activities are confined near the subsurface region close to the indenter in the case of Ni$_3$Al systems while dislocation loops propagate into the substrate in the NiAl systems.

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