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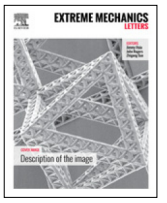

Crack healing in nanocrystalline palladium

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ABSTRACT

We present molecular dynamics simulations that demonstrate crack healing induced by external mechanical loading in three-dimensional models of nanocrystalline palladium. This behavior is due to the interaction of a crack with internal stresses in the surrounding microstructure. Our observations illustrate the importance of accounting for microstructurally-induced internal stresses when predicting the behavior of nano-scale cracks under mechanical loading. They also motivate further work to determine whether internal damage in hard matter may be mitigated by designing microstructures that heal cracks during mechanical loading.

Internal damage is life limiting for many functional and structural materials subjected to mechanical, thermal, or electrochemical loading [1,2]. Living organisms have adapted to heal internal damage. An analogous ability to self-heal would improve materials performance in a broad range of technologies, including energy, transportation, and infrastructure applications. Biologically inspired mechanisms for self-healing have received considerable attention in soft matter [3,4], where self-healing has been pursued through incorporation of encapsulated healing agents [5], chemically assisted polymer network reconstruction [6], or local melting and flow [7]. However, these mechanisms are largely not applicable to hard matter, such as metals or ceramics, prompting several recent investigations into non-biological self-healing mechanisms [8–11]. In this letter, we demonstrate crack healing in molecular dynamics (MD) simulations of mechanically loaded nanocrystalline palladium (nc-Pd).

On the macroscale, "damage" in materials always refers to a deterioration of desirable properties. However, damage may be connected to a wide range of structures on the microscale, such as voids [12] and precipitates [13], interfaces depleted of or enriched in certain elements [14], bands of flow localization [15,16], states of free surfaces [17,18], and many others. Here, we focus on one specific type of damage: the incipient crack. Incipient cracks are gaps or rifts in a material that are well below the critical size required for unstable crack growth under a given external loading condition. In some cases, they are little more than high aspect ratio oblate cavities or "microvoids" [19]. However, incipient cracks play an important role in potentially life-limiting material failure processes, such as fatigue [1,20]. They have therefore been studied extensively, both in experiments [21–23] and in simulations [19,24,25]. The ability to heal them may extend the lifetime and reliability of structural and functional materials.

Compressive loading is expected to close cracks, providing an opportunity for them to bond and heal. Surprisingly, monotonic shear and even tensile loading may also give rise to mechanically driven crack healing, provided that the loading generates non-uniform internal stresses that give rise to local compression near the crack [8,9]. In previous MD simulations of model two-dimensional (2D) nonperiodic microstructures, we showed that stress-driven grain boundary migration [26–28] may lead to crack tip compression and, in some cases, crack healing [8]. Thus,

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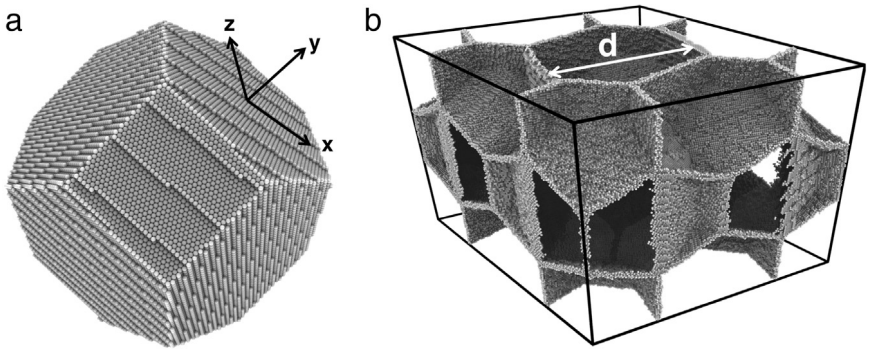

Fig. 1. (a) A crystalline Pd grain shaped as a truncated octahedron. (b) The nc-Pd model used in the present study. For clarity, atoms with perfect face-centered cubic (fcc) environments are not shown.

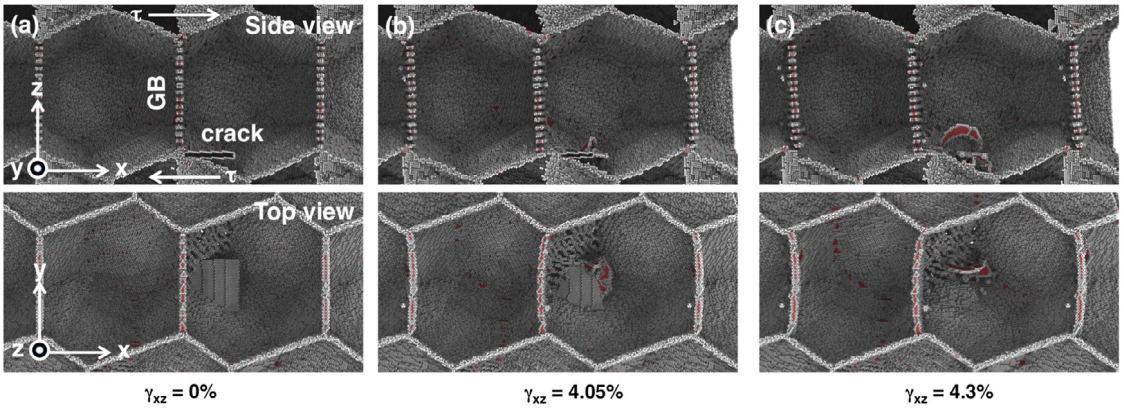

Fig. 2. Simulation of a crack in nc-Pd during shear loading. The top row shows the crack edge-on while the bottom row shows it in plan-view. Applied strains are indicated below the figures. For clarity, atoms with perfect fcc environments are not shown. (a) Initial model structure. (b) Upon shearing, the crack begins to close at its right end (far from the GB). (c) Eventually, the crack heals completely.

crack behavior is coupled to the microstructure and its evolution through internal stresses. In this work, we further investigate mechanically driven crack healing in more realistic, fully three-dimensional (3D) periodic microstructures of nc-Pd using large-scale MD simulations.

We build a model 3D nc-Pd grain structure composed of uniform, space-filling truncated octahedra of width $d = 20$ nm, measured between two opposing hexagonal faces, as illustrated in Fig. 1. Similar models have been previously used in studies involving 3D grain structures [29,30] and are a reasonable representation of nc-Pd created by consolidation of Pd nanoclusters synthesized through inert gas condensation [31]. Of the five convex polyhedra that tessellate 3D Euclidean space [32,33], truncated octahedra do so with least interface area per unit volume [34], resulting in models with lower total grain boundary (GB) energy than microstructures generated with the more commonly used Voronoi construction [35,36]. Our model contains two grains along each cell direction (i.e., $2 \times 2 \times 2 = 8$ grains, total). Thus, the periodic images of GBs along any cell direction form a sequence of boundaries of identical plane orientation and misorientation axis as well as misorientation angles of equal magnitude, but alternating sign.

We carry out MD simulations using LAMMPS software [37] and an embedded-atom method (EAM) potential for Pd [38]. Our model has dimensions 40 nm × 40.8 nm × 35.4 nm with periodic boundary conditions applied in all directions. It contains ∼4.25M atoms. We introduce a 7.5 nm × 7.5 nm square-shaped crack of thickness 1 nm in the vicinity of one of the GBs by removing atoms, as shown in Fig. 2(a). The thickness of the crack is larger than twice the cutoff radius of our EAM potential [38], which guarantees that the crack is stable at zero stress. We apply external loading by iteratively shearing the supercell by $\gamma_{xz} = 0.1\%$ followed by 5 ps of MD relaxation after each strain increment, yielding an average strain rate of 2×10^8/s. Temperature is kept fixed at 10 K using a Nosé–Hoover thermostat [39,40].

Fig. 2 shows the effect of loading on the crack in nc-Pd: the crack progressively closes, even though the applied strain is simple shear and has no net compressive component. At an average shear strain of $\gamma_{xz} = 4.05\%$, the crack surfaces far from the GB touch and bond (see Fig. 2(b)). Concurrently, Shockley partial dislocations with $[1\bar{1}2]$ Burgers vectors nucleate from the crack faces where bonding occurs. They are followed by trailing partials with $[21\bar{1}]$ Burgers vectors. The emitted dislocations have net Burgers vectors perpendicular to the crack surfaces, consistent with crack closure. At an average shear strain of $\gamma_{xz} = 4.3\%$, the nanocrack bonds along the entirety of both of its surfaces and is completely healed (see Fig. 2(b)). Further loading leads to nucleation of dislocations at GB triple

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