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Design of fracture-resistant silicon structure with molecular dynamics simulation

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ABSTRACT

The inherent brittleness of crystalline silicon is a cause of concern for processing, handling and application of the material. Here a simulation-based design is proposed to reduce the risk of catastrophic brittle fracture of devices and components made of silicon. In this scheme, ultrathin layers of amorphous silicon are introduced within the crystalline silicon to create a multilayered laminated structure. Using molecular dynamics simulations, we demonstrate that in this nanolaminate, a crack growing within the crystalline region gets pinned at the amorphous layers. This phenomenon occurs due to the observed ductility in amorphous silicon, which resembles the shear-band mediated deformation of metallic glasses. As a consequence, the catastrophic failure is averted by localizing the damage and preventing it from extending across the material.

1. Introduction

Over the last several decades, silicon has become almost synonymous with modern technology. With the advent of information age, instead of remaining confined within the scientific community, name of this wonderful material has gained a more exoteric identity. Despite its immense technological importance, silicon is extremely brittle below a temperature of about 800 K [1]. As a matter of fact, it is often used as an ideal brittle solid for investigating the fundamental aspects of fracture mechanics. This poses significant challenges to engineers who intend to deploy it in conditions where the risk of its catastrophic failure is high. This problem is particularly severe in applications, where silicon is used to fabricate high-speed micromechanical components like gears and turbines [2]. Recently, on account of its favorable properties [3,4], several manufacturers have started producing mechanical watches made of Si parts. In such a scenario, not many pragmatic options are available to reduce the inherent brittleness of Si without increasing the operational temperature. Reducing the size to nanoscale is found to enhance its ductility [5]; however, from a practical standpoint, it is seldom possible to replace a macroscopic, or even a micro-sized sample, with its nanosized counterpart. Similarly, artificial surface nanotexturing has been shown to be an effective method for making fracture-resistant Si devices [6]. Although this technique is capable of reducing the stress concentration at a crack-tip in vicinity of the surface, it is ineffective against a crack originating deep inside the solid. Therefore, if Si components form parts of a larger composite system, they continue to be regarded as the weakest link in terms of the overall mechanical strength of the structure.

Aiming to address the above-discussed issue, we propose a simple structural manipulation to reduce the brittleness of Si components. This design involves introduction of ultra-thin layers of amorphous silicon (a-Si) within the crystalline material. Thus, a nanolaminated structure consisting of alternate layers of crystalline and amorphous silicon would be obtained. Recently, Fuentes-Edfuf et al. [7,8] have demonstrated that patterned microstructure consisting of alternate amorphous-crystalline regions can be created by exposing crystalline silicon to ultrashort laser pulses. In our proposed multilayered structure, a crack nucleated in a crystalline layer can grow only if it passes through the adjacent amorphous layers without any hindrance. Sung and Chen [9] have performed atomistic computations to explore the effect of quenching rate on the fracture behavior of NiAl alloy. It was observed that a glassy state was obtained upon very fast quenching, while reducing the quenching rate resulted in partially crystalline alloys with amorphous grain boundaries. In samples with large degree of amorphization, improved ductility was observed owing to the phenomenon of crack-tip blunting. Besides the metallic alloys, composite systems with amorphous phases have also been studied in the context of carbon-based materials. For instance, the composites made of carbon nanotubes and amorphous carbon have been shown to possess enhanced wear and

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fracture resistance [10,11]. Similarly, the coating of amorphous carbon on SnO_2 nanowire is found to resist the fracture due to lithiation [12]. In particular, the comparative study by Lu et al. [13] have revealed that in stark contrast to diamond where catastrophic fracture takes place, the amorphous form of carbon shows a ductile-like behavior. Owing to the similarities in terms of crystal structure and nature of bonding, we can heuristically draw parallels between diamond and silicon. Hence, in the case of our proposed laminated structure, one may hypothesize the possibility of having different trends of crack-tip dynamics in the crystalline and amorphous Si layers. A number of experimental studies have indicated improved fracture-toughness of laminated structures composed of alternate layers of brittle and ductile solids. The efficacy of this method has been demonstrated for different types of multi-layered materials. For instance, Launey et al. [14] have reported the biomimetic design of ceramic-metal composites with improved performance. Similarly, the laminates made of brittle layers of Nb_3Al and ductile layers of Nb are found to have excellent fracture-resistance [15]. In all such studies, the fracture-prone layer is typically a ceramic or brittle metal, while the ductile layer consists of a ductile metal. If the amorphous silicon is indeed found to exhibit enhanced ductility, we can in principle, apply the same idea to design a laminated Si structure where the a-Si can form the ductile layer. Hence, the proposed structure is of particular interest as both brittle and ductile layers have the same chemical composition. This feature, which is not present in the other brittle/ductile multi-layered systems studied previously, attributes uniqueness to the amorphous-crystalline silicon nanolaminate studied here.

In the present study, we employ molecular dynamics (MD) computations to test the validity of the proposed structure. The tool of atomistic simulation is particularly relevant here, for sufficient experimental data regarding the mechanical behavior of a-Si is not available. In addition, MD provides a comprehensive insight into the underlying mechanism of a process at atomistic scales of length and time, which are difficult to access with other methods. This is why, in the context of fracture in solids, MD simulations have been successfully used to explore several fundamental aspects like brittle to ductile transition [1], crack-tip velocity [16], effects of point defects [17] and reinforcements [18], cohesive-zone modeling [19,20], etc. The scheme of simulation followed in this work involves a two-step investigation. In the first step, we study how a crack grows in pure a-Si under applied tensile load. This simulation is carried out at three different temperatures in order to observe the temperature-effect on the nature of fracture. Once the plastic deformation behavior of a-Si is established, we are able to predict the performance of the proposed crystalline-amorphous multilayered composite. In the next step of computation, this prediction is tested directly through a separate set of simulations, which enables us to comprehend the interaction between the crack-tip and amorphous silicon layer.

2. Computational details

We first investigate the modality of crack-propagation in amorphous Si at different temperatures. To this end, a crystalline block of Si is created with dimensions of about 45 nm × 15 nm × 1.6 nm, with periodic boundary condition in all the three directions. The crystal is melted at a temperature of 2500 K and rapidly quenched to 10 K at a rate of 50 K/ps. During this process, the temperature is controlled by the Nosé-Hoover thermostat [21,22], while the simulation cell is allowed to dilate or shrink in order to maintain zero pressure on the system. This cycle of heating and quenching is repeated several times to obtain a homogeneous amorphous phase. Finally, the system is subjected to structural relaxation under zero hydrostatic stress through conjugate gradient method to attain the minimum energy configuration. As the simulation cell is very thin and periodic along the *z*-direction, we may consider this as a quasi-2D computation. Once the amorphous sample is created, a small elliptical crack of dimensions 4 nm × 1 nm is introduced at the center of the simulation cell (see Fig. 1(a)). The final structure of the amorphous plate consists of 56,290 atoms. This amorphous plate with the initial crack is thermalized and strained along the vertical direction at a rate of $\sim 7.5 \times 10^8\ s^{-1}$. Simulations are carried out at 50 K, 300 K and 500 K temperatures.

As mentioned in the introductory section, our proposed laminated structure consists of nanosized layers of a-Si separating the crystalline regions. To implement this idea, we create a quasi-2D crystalline Si slab of size 120 nm × 40 nm × 1.6 nm and orientation $\langle 112\rangle \times \langle 11\bar{1}\rangle \times \langle 1\bar{1}0\rangle$. At the center of the simulation cell, atoms are removed from two successive atomic planes normal to the *y*-direction to introduce a narrow crack which extends about 3 nm along the *x* direction. In order to create the amorphous layers, two thin strip-like vertical regions separated by 20 nm are selected on both sides of the crack. The repeated melting-quenching process used to obtain the previous amorphous sample (Fig. 1(a)) is used here also, but only the atoms belonging to the two thin regions undergo this process while the rest of the atoms are kept frozen. At the end of simulation, we obtain two amorphous layers on both sides of the crack as demonstrated in Fig. 1(b), where the atoms are colored according to their local crystal structures estimated through a modified form of the common neighbor analysis [23]. It is possible to change the widths of these layers by altering the corresponding widths of the melt-quench regions. Accordingly, structures with layer-thicknesses of 2 nm, 3 nm, 4 nm and 8 nm have been produced and used in this study. All the nanolaminated slabs have 371,456 Si atoms.

The tensile deformation of the purely amorphous sample (Fig. 1(a)) is primarily intended to observe the fundamental crack-tip behavior at different temperatures and hence, only a crude simulation setup is employed for the purpose. In contrast, we use a more elaborate and refined method for the deformation of the crystalline-amorphous Si nanolaminate, so that the effects of stress waves and direct thermostat-interference can be minimized. In this method which is schematically presented in Fig. 1(c), the system is spatially partitioned into several regions and during the MD time-integration, different modes of dynamics are imposed on the atoms in those regions. Following is the brief description of different types of dynamics followed by the atoms.

Fixed atoms – Atoms belonging to two thin layers (red[1] colored atoms in Fig. 1(c)) at the top and bottom of the system are kept fixed during the simulation. This is implemented by zeroing out the forces and initial velocities of these atoms.

Damped atoms – The blue colored atoms shown in Fig. 1(c) constitute the damping regions. Here each atom experiences a damping force proportional to its velocity, i.e., $F = -\gamma v$. In these simulations, a value of 0.2 eV ps/Å^2 has been selected as the damping coefficient γ. During fracture, a crack-tip emits stress waves [24,25], which may get reflected by the top and bottom layers of fixed atoms. In addition, stress waves generated in the periodic image cells can also enter the primary simulation cell. As the interaction between a crack-tip and stress wave can affect the behavior of crack-propagation [26], we need to minimize this spurious effect arising out of the artifacts of MD setup (finite size and periodic boundaries). Here the damped atoms cater to this need by absorbing the kinetic energy associated with the stress waves [27],

[1] For interpretation of color in Figs. 1 and 5, the reader is referred to the web version of this article.