Molecular Dynamics Investigation on the Phosphorus Doping Effects on the Mechanical Properties of Crystal Silicon

Bin Liu\textsuperscript{1,a,}, Yangjiao Li\textsuperscript{1,b}, Yingjuan Yue\textsuperscript{1,d}, Yi Tao\textsuperscript{1,c}, Zhongbao Qin\textsuperscript{1,e} and Chen Cheng\textsuperscript{1,f}

\textsuperscript{1}Rocket Force University of Engineering, 403 Department, Xi’an, China

\textsuperscript{a}liubinbin19880108@163.com, \textsuperscript{b}lyjxjtu@126.com, \textsuperscript{c}yingjuanyue@163.com, \textsuperscript{d}wanfangzhang_1979@163.com, \textsuperscript{e}zhongbao_qin@163.com, \textsuperscript{f}cche943@sina.com

*Corresponding author

Keywords: Crystal Silicon, Phosphorus, Modified Embedded Atom Method, Molecular Dynamics, Mechanical Properties.

Abstract. The effects of phosphorus (P), one of the most common impurities in silicon (Si), on the mechanical responses of crystal Si (c-Si) under tension are investigated using molecular dynamics with a Modified Embedded Atom Method (MEAM) potential. Tensile tests at 300K are applied for bulk c-Si with uniformly distributed and aggregated P impurities, notched c- Si films with P doping on the crack tip or at the middle of the crack propagation path. For bulk c-Si, local defects come into being around P, then rapidly nucleate and propagate, finally lead to brittle fracture. The fracture threshold decreases as the concentration increases, no matter P atoms are uniformly distributed or regionally aggregated. However, for notched c-Si film, P can evidently enhance its fracture strength by blocking the origin and propagation of cracks. With regard to Si-based micro/nano structures, fracture usually starts from the surface, indicating that P impurities play a critical role on the surface.

1. Introduction

Pure elementary silicon (Si) when doped with traces of elements such as phosphorus (P) is an important semiconductor material, which has been extensively applied in high-tech industries like integrated circuit (IC), micro/nano-electro-mechanical systems (MEMS/NEMS), solar cells and so on. Besides, as a representative covalent material, it is attractive in fundamental physics. Phosphorus(P) not only is the electrical activation factor of Si, but also imposes effects on its mechanical\cite{1-4} and thermal\cite{5} properties. The mechanical failures like high acceleration shock, fatigue fracture, etc. of Si-based micro/nano cantilevers\cite{6}, multi-axis accelerometers\cite{7} etc., have drawn much attention recently\cite{8, 9}. The special role that impurities play in the failures of Si-based structures is worth studying.

Doping with foreign atoms is an effective way to modify materials properties\cite{10, 11}. Up to now, lots of experiments about how P affects the mechanical properties of Si have been performed. Some yield contradictory results owing to complicated experimental conditions. For instance, Cook et al.\cite{12} reported that heavy P doping at a level of 10^{-18}-10^{-19}cm^{-3} exhibited no clear influence on the fracture toughness of Si, and Nagy et al.\cite{13} showed that ion implanted P increased the Young’s modulus of single crystal Si, while Zeng et al.\cite{1} declared that the fracture toughness and Young’s modulus were, respectively, increased and decreased by heavy P doping at ~5×10^{19}cm^{-3}. First principle calculations\cite{14, 15} predicted a reduction in ideal tensile strength by heavy doping at
~$10^{21}$ cm$^{-3}$, while our recent experiments[16] showed an statistical increment of bending strength by heavy doping at ~$10^{19}$ cm$^{-3}$. It is worth mentioning that the defects in P-doped specimens introduced by processing techniques, like ion implantation and heat spreading, bring uncertainties to post-test analysis. Therefore, to clarify the underlying mechanism, insights into the microcosmic processes are necessary. To this end, computational method is an excellent option as it enables atomic or nano scale investigation on materials properties.

Quantum mechanics-based density functional theory (DFT) and molecular dynamics (MD) are currently the most extensively used computational techniques. DFT provides the most reliable information, which, however, is incapable of dealing with a thousand-scale system despite the rapid development of computer technologies. Somehow, many physical phenomena, like defect nucleation, can be only observed in large systems. (Semi-)Empirical potentials have developed enormously in recent decades and can enable the simulation for million-level systems. The reliability of MD results largely depends on the interatomic potentials. A semi-empirical model Modified Embedded Atom Method (MEAM) is used in the current work, which was constructed by Baskes et al.[17] by adding angular terms to EAM formalism[18], and has been extensively applied in a wide range of fields. Currently, 26 elements have been covered by MEAM[19] including metal materials, semiconductors, gas elements like nitrogen, oxygen, hydrogen, which shows the universality of MEAM formalism. Recently, Lee and Baskes developed a more generalized version, namely second-nearest-neighbor MEAM (2NN MEAM).

Only a few empirical potentials for Si-P binary system can currently be referenced. Lee et al.[5] developed a SW potential for Si-P binaries to better describe the effects of P on the thermal conductivity of Si. Wilson et al.[20] investigated the diffusion of P on the surface of Si crystal using Environment Dependent Interatomic Potential (EDIP) model. However, these two potential formalisms are not suitable for fracture simulation since they fail to maintain the brittleness of Si. Though the SW potential modified by Hauchet et al.[21] can yield brittleness, it is not reliable since many other important properties such as elastic constants are unacceptably predicted. Comparatively, MEAM maintains the brittle nature of Si[22-25]. Up to now, Si-based multi-element MEAM potentials include Si-Ni[26], Si-Li[27], Si-Al/Fe/Cu/Mg[28], while that for Si-P is still unavailable. According to Mattila’s work[29, 30] that EAM model can be used for P-based system, MEAM can accordingly also be applied to describe systems containing P. We have recently developed a 2NN MEAM potential for Si-P binary system using genetic algorithm (GA) based on a wide variety of fundamental physical properties from experimental data and high-level calculations[31].

In this study, our recently developed 2NN MEAM potential is used to investigate the effects of P on the tensile mechanical responses of bulk, notched crystal Si, and bulk and film a-Si. We aim to clarify the underlying physical mechanism and provide suggestions for processing technologies.

2. Methodology

In (2NN) MEAM formalism, the total energy of a system is calculated in the following equation:

$$E = \sum_i \left[ F_i(\vec{p}_i) + \frac{1}{2} \sum_{j \neq i} \phi(R_{ij}) \right]$$

(1)
where $F_i(\tilde{\rho}_i)$ is the embedding function, $\tilde{\rho}_i$ is the background electron density at site $i$, and $\phi(R_{ij})$ is the pair interaction between atoms $i$ and $j$ at a distance $R_{ij}$.

We use Lee’s 2NN MEAM parameter set for pure Si[32]. 2NN MEAM potentials for pure P and Si-P binary system have been developed in our recent work[31]. In order to produce a reliable potential to describe Si-P compounds, a variety of fundamental physical properties are considered, including cohesive or formation energies, lattice constants and elastic constants of typical Si-P structures, properties of point defects and P-vacancy pairs.

All the calculations in present work are performed using Large-scale Atomic/ Molecular Massively Parallel Simulator (LAMMPS)[33]. The simulations aim to reveal the mechanism on how P influences the behaviors of fracture, crack generation, nucleation and propagation of c-Si.

Two types of specimens are prepared for tensile tests of c-Si, namely bulk models and notched films, which are respectively used to investigate how P affects the mechanical behaviors when sited evenly in bulk Si and at the crack tip or crack propagation path in notched Si films. Correspondingly, the periodic boundary conditions (PBC) are applied in three dimensions for the former, and $z$-dimension for the latter. As for P doped bulk a-Si, three directions are set periodic, and $x$- and $z$-dimensions are periodic in P doped a-Si films. Loading directions are all along $x$-dimension. All the tensile tests are conducted at constant temperature 300K and pressure 1bar by means of Nosé-Hoover thermostat[34] and Parrinello-Rahman pressostat[35], i.e. NPT ensemble. In all cases, before loading, the models are relaxed for 100ps to remove the stresses that can develop due to thermal expansion or surface reconstruction. The strain rate is $5 \times 10^7$ s$^{-1}$ for bulk crystal models and $10^8$ s$^{-1}$ for the others.

3. Effects of P doping on the mechanical response of c-Si under uniaxial tension

3.1 Effects of P doping concentration on the tensile properties of bulk c-Si.

Three tensile loading directions are considered, i.e. $[1\ 0\ 0]$, $[1\ 1\ 0]$ and $[1\ 1\ 1]$. The corresponding right-handed axes $y$ and $z$ are schematically shown in Fig. 1. The specimens are prepared by substituting Si atoms with P atoms uniformly in crystal Si, i.e. one P atom in the central position of every $N \times N \times N$ (integer) unit cell, where different $N$ corresponds to different concentration. The model sizes and atomic numbers for $[1\ 0\ 0]$, $[1\ 1\ 0]$- and $[1\ 1\ 1]$-tension models are $65.17 \times 65.17 \times 32.59$ Å and 6912, $53.76 \times 46.08 \times 43.45$ Å and 5376, $56.44 \times 38.40 \times 53.21$ Å and 5760, respectively. The models are not constructed by randomly distributing the P impurities as physical reality simply because of the uncertainty that random distribution can introduce to the results. In the case of random distribution, we have to run several times for each concentration in order to see a clear trend about how P affects the tensile response of bulk Si. Besides, random distribution might introduce regional high concentration that can make the results difficult to explain. Present work has only done the tensile tests of randomly distributed $[1\ 0\ 0]$-tension models to illustrate that the concentration shows a similar manner to uniform distribution models.

Fig.1(a)~(c) plot the stress-strain curves of P doped Si strained along different orientations. The reduction of the tensile fracture threshold as P doping concentration increased can be easily observed. The lattice distortion introduced by substitutional P atoms evolves into local defect, then nucleates and propagates when the strain is high enough, consequently leading to brittle fracture. To illustrate this process, take the $[1\ 1\ 0]$-tension model with the concentration of 0.298% (corresponding to the black curve in Fig.1(b)) for instance, the configuration evolution is shown in...
Fig. 5(a)~(d). The snapshots are visualized by Ovito[36]. It can be easily seen that the micro-void originates around P then nucleates into crack.

Two aspects concerning Fig. 1 are noteworthy. First, the incremental discontinuity of stress can be observed in the case of [1 0 0]-tension model with the concentration of 0.463% at around 0.20, see Fig. 1(a). This is due to that the P atoms are noticeably displaced from their lattice positions to release local high strain energy. A similar phenomenon has been reported in the nano-indentation behavior of Si[37], which is called “pop-in”. Second, there exist jagged parts of the curves in the case of [1 1 0] models. It is found that the close packed atom sets slide on inclined planes when intensively strained, as the black arrows indicate in Fig. 2(b). However, the slip is supposed to be continuous as the increment of strain is smooth. When the shear stress exceeds the threshold value, the slip is activated and the atoms should be immediately rearranged to preferred positions, not in jagged manner. According to our recent research[24], this is due to the intrinsic drawback of the MEAM potential for Si as the general stacking fault energy (GSFE) curves in shuffle (1 1 1) plane is not smooth. The slip cannot be reactivated when strain reaches ~0.17, which is probably due to the reason that the threshold of the remapped configuration under high strain is too large to overcome before fracture.

![Figure 1. Tensile stress-strain curves of c-Si with different orientations. (a) loading direction x-[1 0 0], (b) loading direction x-[1 1 0], (c) loading direction x-[1 1 1]. Different color corresponds to different P concentration. The right-handed axes x, y and z are schematically shown in each figure.](image1)

Tensile test results of [1 0 0]-tension models with randomly distributed P impurities are shown in Fig. 2. Model construction and following tensile test are repeated five times for each concentration. One can easily see the uncertainty of fracture threshold and the overall decreasing trend, and that the fracture thresholds of uniformly distributed models are evidently larger than those of randomly distributed ones, probably due to higher regional concentration. It is expected to repeat the tests several times to see an obvious trend, consequently bringing much more computation burden. Replacing a Si atom by a P atom periodically in every \(N \times N \times N\) unit cell won’t bring such uncertainty, which is an ideal model as foreign P atoms wouldn’t array periodically in physical realities. However, both of these two kinds of models yield descending trend as the concentration increases.

![Figure 2. Comparison of tensile test results between [1 0 0]-tension models with randomly and uniformly distributed P impurities. In the case of random distribution, model construction and tensile test are repeated five times for each concentration. One can observe the uncertainty of fracture threshold introduced by random distribution and the overall decreasing trend. The fracture thresholds of uniformly distributed models are evidently larger than those of randomly distributed ones, which is probably due to the regional high concentration.](image2)
3.2 Effects of impurity aggregation on the tensile properties of bulk c-Si.

In this part, the models are constructed by symmetrically replacing eight Si atoms with P atoms. The sizes, number of atoms (concentrations) for [1 0 0]-, [1 1 0]- and [1 1 1]-tension models are 32.59Å×32.59Å×32.59Å and 1728 (0.463%), 53.76Å×46.08Å×43.45Å and 5376 (0.149%), 56.44Å×38.40Å×53.21Å and 5760 (0.139%), respectively. The distances between them are shown in Fig. 3(a). The axes combination and simulation setup are the same as Part 3.1. The tensile curves are plotted in Fig. 3, where the blue curves are from uniformly distributed models. One can see that the fracture threshold declines as the P atoms aggregate, i.e. the local concentration gets higher. The probable explanation can be stated as follows. The lattice distortion introduced by P atoms enlarges as strain increases. The radius of the largest distortion region right before fracture is about 7Å. When P atoms are close enough, the distortion regions overlap and interact, accelerating the generation of regional micro-voids, thus making it easier to fracture.

Fig. 3 Tensile stress-strain curves of the models with different loading directions and local P doping concentrations. (a)loading directions x-[1 0 0], the purple balls stand for P atoms, a, b and c are the sizes of the rectangle enclosed by 8 P atoms, in Å, (b)loading direction x-[1 1 0], (c)loading direction x-[1 1 1].

From above discussions, we can conclude that the tensile fracture strength of bulk Si decreases as the P doping concentration increases, no matter uniformly distributed or locally congregated. This is consistent with the first principle calculations by Huang et al.[14, 15]. However, our recent experiments[16] show an statistically rising trend of the bending strength of micro-beams as the concentration increases. It seems that our MD calculations and experiments are contradictory. But the model used for MD calculation is bulk and has no surface effect which is dominant in controlling the fracture of micro/nano structures. Therefore, only when how P affects the origin and propagation of cracks is clarified can one make the judgment about whether P strengthens or weakens the fracture behaviors of Si.

3.3 Effects of P doping on the mechanical response of notched c-Si films.

The principal cleavage planes in crystal Si are {1 1 0} and {1 1 1}[38-42]. In present research, cleavage fracture is simulated using three types of crack system {1 1 0}<1 1 0>, {1 1 1}<1 1 0> and {1 1 1}<2 1 1>. The sizes in three dimensions and number of atoms are 174.73Å×136.33Å×21.72Å and 25912, 140.32Å×136.33Å×26.61Å and 25312, 140.32Å×133.03Å×30.72Å and 28192, respectively. Two doping patterns are designed, one with P doped notch tips, the other with P sited in the middle of the crack propagation path. PBC is applied in z-dimension. The strain rate is 10^8 s^{-1}.

Fig. 4 presents the stress-strain curves. By comparing the curves of pure Si and P doped models, we can see that the cracking of P doped notch tip films happens at higher strain compared with that of pure Si films, and that the crack propagation of middle doped films is obviously blocked by P dopant as the stress rebounds. To give a concrete description of the blocking, take the black curve in Fig. 4(a) for example, the snapshots corresponding to each inflection point are shown in Fig. 5(c)~(g). Fig. 5(h) shows the configuration after fracture.
Figure 4. Effects of P doping on the tensile mechanical response of notched Si. (a) x-[1 1 0], y-[1 -1 0], z-[0 0 1], the cyan balls stand for P atoms, (b) x-[1 1 1], y-[1 -1 0], z-[1 1 -2], (c) x-[1 1 1], y-[2 -1 -1], z-[0 1 -1], loading directions are all along x. Three cases are compared, pure Si, P doped in the middle of crack propagation path, and P doped notch tip. The atomic models are given to graphically show the doping patterns. The stress rebound in the curves caused by stress barrier is wiped out in order to highlight the effects of crack propagation blocking except [1 1 1]<2 1 1> with P doped crack tip.

Figure 5. Structural evolution before and after the fracture of [1 1 0]-oriented model. (a)~(d) respectively show the configurations of 0.298% P doped model before tension, P-induced defect nucleation, crack propagation, and after fracture. (e)~(g) are corresponding to the inflection points of the black curve in Fig. 4(b), (h) is the snapshot after fracture, the strains for each snapshot are respectively 4.86%, 4.96%, 6.54% and 6.58%. The defects in bulk model nucleate then evolve into a crack and propagate at the strain of about 22.35%(c), which is obviously larger than the cracking strain of notched model, 4.86%.

The fracture discontinuity is note-worthy, see the light blue part following the red curve in Fig. 4(c). This is caused by intrinsic shortcoming of the potential[24, 42]. When the films break, i.e. the fracture surfaces are generated, an artificial stress barrier needs to be overcome to get completely apart. For bulk models, the accumulated strain energies are high enough to overcome the stress barrier, thus without stress rebound. For notched ones, the strain energy is not enough when fracture happens so that extra strain energy needs to accumulate to get over the barrier. Details can be found in our recent paper[24]. The stress rebound in stress-strain curves caused by stress barrier might mislead readers. Hence, the stress rebounds by artificial stress are wiped out in Fig. 4, in order to highlight the effects of crack propagation blocking (the blue part in Fig. 4(c) is shown just to illustrate above explanations).

At room temperature, the bond strength of P-P (489.5±10.5kJ/mol) and Si-P (363.6kJ/mol) are higher than that of Si-Si (325±7kJ/mol)[43]. We have also calculated the bond strengths of P-P (413.87kJ/mol), Si-P (371.09kJ/mol) and Si-Si (302.99kJ/mol) using MEAM. Though the MEAM predicted bond strength of P-P exhibits larger error, the bond strengths of three bond types
calculated by MEAM share the same order as experimental values. The bonds with higher strength are more difficult to break, theoretically supporting our simulation results.

Here naturally arises the question why the strength of bulk c-Si declines when doped with P since the bond strengths of P-P and Si-P are larger than that of Si-Si. As explained above, the local distortion caused by P atoms can easily develop into local defect when sufficiently strained. Strain energy tends to be released through defects. So before fracture, the accumulated strain energy of bulk P doped c-Si is less than that of pure bulk c-Si, i.e. the fracture strain of the former is smaller. Considering the stiffness is negligibly changed, the fracture threshold of the former is smaller.

By comparing Fig. 4 with Fig. 1 and Fig. 3, we can see that the notched models fracture obviously earlier than that of bulk models because of the huge stress concentration at the crack tip. In crystal Si micro/nano structures, the mechanical failure practically starts from the defects on surface. In this manner, P atoms on surface, especially near the defects, produce effects earlier than those inside the crystal. Besides, though the cracking of the notch can be blocked by P atoms, as the strain keeps ascending, the cracking will continue before the cracking around the P atoms inside the crystal starts. Take the [1 1 0]-tension model as example (see Fig. 4(a)), the cracking of notched model starts at strain 5.1% which is much smaller than that of bulk model, 22.3%. Overall, P impurities strengthen Si micro/nano structures by impeding the cracking and blocking the propagation of pre-existing notches.

4. Summaries

The main contribution of this work is clarification of how P doping influences the mechanical properties of c-Si using a recently developed 2NN MEAM potential for Si-P binary system. The potential is proved to be reliable for simulating the mechanical response of Si-P system since our results are in accordance with Ref.[14] on the reduction of the tensile threshold of bulk Si, and with Ref.[16] on the enhancement of the tensile strength of notched Si. The results are summarized as follows. (1) The tensile fracture stresses of bulk Si is obviously decreased by P impurities. The reduction of stiffness is not as apparent as fracture stresses. (2) Dopant P can effectively block the cracking of defects on surface and block the propagation of cracks. This effect plays a dominant role in strengthening the mechanical properties of Si-based micro/nano structures.

5. Acknowledgement

This work is financially supported by National Natural Science Foundation of China (No. 51705522), and Young Talent fund of University Association for Science and Technology in Shanxi, China (No. 20180412).

References

[1] Z. D. Zeng, X. Y. Ma, J. H. Chen, Y. H. Zeng, D. R. Yang, and Y. G. Liu. Effects of heavy phosphorus-doping on mechanical properties of Czochralski silicon[J]. *Journal of Applied Physics*, vol. 107, 2010.

[2] H. D. Chiu. Phosphorus concentration limitation in Czochralski silicon crystals[J]. *Journal of the Electrochemical Society*, vol. 147, pp. 345-349, 2000.

[3] H. Siethoff, and H. G. Brion. The interaction of boron and phosphorus with dislocations in silicon[J]. *Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing*, vol. 355, pp. 311-314, 2003.
[4] Y. Ohno, T. Shirakawa, T. Taishi, and I. Yonenaga. Interaction of phosphorus with dislocations in heavily phosphorus doped silicon[J]. *Applied Physics Letters*, vol. 95, 2009.

[5] Y. Lee, and G. S. Hwang. Mechanism of thermal conductivity suppression in doped silicon studied with nonequilibrium molecular dynamics[J]. *Physical Review B*, vol. 86, 2012.

[6] H. K. Liu, C. H. Pan, and P. P. Liu. Dimension effect on mechanical behavior of silicon micro-cantilever beams[J]. *Measurement*, vol. 41, pp. 885-895, 2008.

[7] S. S. Nasiri, and J. Seeger, *Multiple axis accelerometer*. 2007, Google Patents.

[8] S. Yoneoka, Y. Q. Qu, S. S. Wang, M. W. Messana, A. B. Graham, J. Salvia, B. Kim, R. Melamud, G. Bahl, and T. W. Kenny. High-Cyclic Fatigue Experiments of Single Crystal Silicon in an Oxygen-Free Environment[J]. *Mems 2010: 23rd Ieee International Conference on Micro Electro Mechanical Systems, Technical Digest*, vol. pp. 224-227, 2010.

[9] M. Sheehy, J. Punch, S. Goyal, M. Reid, M. Lishchynska, and G. Kelly. The Failure Mechanisms of Micro-Scale Cantilevers Under Shock and Vibration Stimuli[J]. *Strain*, vol. 45, pp. 283-294, 2009.

[10] B. Mortazavi, and S. Ahzi. Molecular dynamics study on the thermal conductivity and mechanical properties of boron doped graphene[J]. *Solid State Communications*, vol. 152, pp. 1503-1507, 2012.

[11] B. Mortazavi, S. Ahzi, V. Toniazzo, and Y. Remond. Nitrogen doping and vacancy effects on the mechanical properties of graphene: A molecular dynamics study[J]. *Physics Letters A*, vol. 376, pp. 1146-1153, 2012.

[12] R. F. Cook. Strength and sharp contact fracture of silicon[J]. *Journal of Materials Science*, vol. 41, pp. 841-872, 2006.

[13] P. M. Nagy, D. Aranyi, P. Horvath, G. Peto, and E. Kalman. Nanomechanical properties of ion-implanted Si[J]. *Surface and Interface Analysis*, vol. 40, pp. 875-880, 2008.

[14] Y. M. Huang, J. C. H. Spence, and O. F. Sankey. The Effects of Impurities on the Ideal Tensile-Strength of Silicon[J]. *Philosophical Magazine a-Physics of Condensed Matter Structure Defects and Mechanical Properties*, vol. 70, pp. 53-62, 1994.

[15] Y. M. Huang, J. C. H. Spence, and O. F. Sankey. The Effect of Impurities on the Ideal Tensile-Strength of Covalent Crystals - Ab-Initio Quantum Molecular-Dynamics Calculations[J]. *Covalent Ceramics II: Non-Oxides*, vol. 327, pp. 369-374, 1994.

[16] B. Liu, J. Y. Tao, Y. A. Zhang, X. Chen, and X. J. Wang. Effects of phosphorus doping on the bending strength of a single crystal silicon microbeam[J]. *Micro & Nano Letters*, vol. 8, pp. 726-730, 2013.

[17] M. I. Baskes, J. S. Nelson, and A. F. Wright. Semiempirical Modified Embedded-Atom Potentials for Silicon and Germanium[J]. *Physical Review B*, vol. 40, pp. 6085-6100, 1989.

[18] M. S. Daw, and M. I. Baskes. Embedded-Atom Method - Derivation and Application to Impurities, Surfaces, and Other Defects in Metals[J]. *Physical Review B*, vol. 29, pp. 6443-6453, 1984.

[19] M. I. Baskes. Modified Embedded-Atom Potentials for Cubic Materials and Impurities[J]. *Physical Review B*, vol. 46, pp. 2727-2742, 1992.

[20] H. F. Wilson, N. A. Marks, D. R. McKenzie, and K. H. Lee. Molecular dynamics simulations of ion implantation for the fabrication of a solid-state quantum computer[J]. *Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms*, vol. 215, pp. 99-108, 2004.
[21] J. A. Hauch, D. Holland, M. P. Marder, and H. L. Swinney. Dynamic fracture in single crystal silicon[J]. Physical Review Letters, vol. 82, pp. 3823-3826, 1999.

[22] N. P. Bailey, and J. P. Sethna. Macroscopic measure of the cohesive length scale: Fracture of notched single-crystal silicon[J]. Physical Review B, vol. 68, pp. 205204, 2003.

[23] K. Kang, and W. Cai. Brittle and ductile fracture of semiconductor nanowires – molecular dynamics simulations[J]. Philosophical Magazine, vol. 87, pp. 2169-2189, 2007.

[24] B. Liu, H. Zhang, J. Tao, X. Chen, and Y. A. Zhang. Comparative investigation of a newly optimized modified embedded atom method potential with other potentials for silicon[J]. Computational Materials Science, vol. 109, pp. 277-286, 2015.

[25] J. G. Swadener, M. I. Baskes, and M. Nastasi. Molecular Dynamics Simulation of Brittle Fracture in Silicon[J]. Physical Review Letters, vol. 89, pp. 085503, 2002.

[26] M. I. Baskes, J. E. Angelo, and C. L. Bisson. Atomistic Calculations of Composite Interfaces[J]. Modelling and Simulation in Materials Science and Engineering, vol. 2, pp. 505-518, 1994.

[27] Z. W. Cui, F. Gao, Z. H. Cui, and J. M. Qu. A second nearest-neighbor embedded atom method interatomic potential for Li-Si alloys[J]. Journal of Power Sources, vol. 207, pp. 150-159, 2012.

[28] B. Jelinek, S. Groh, M. F. Horstemeyer, J. Houze, S. G. Kim, G. J. Wagner, A. Moitra, and M. I. Baskes. Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys[J]. Physical Review B, vol. 85, 2012.

[29] T. Mattila, R. M. Nieminen, and M. Dzugutov. Simulation of Radiation-Induced Structural Transformation in Glassy Metals[J]. Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, vol. 102, pp. 119-124, 1995.

[30] T. Mattila, R. M. Nieminen, and M. Dzugutov. Simulation of radiation-induced structural transformation in amorphous metals[J]. Physical Review B, vol. 53, pp. 192-200, 1996.

[31] B. Liu, H. Zhang, J. Tao, Z. Liu, X. Chen, and Y. a. Zhang. Development of a second-nearest-neighbor modified embedded atom method potential for silicon–phosphorus binary system[J]. Computational Materials Science, vol. 120, pp. 1-12, 2016.

[32] B. J. Lee. A modified embedded atom method interatomic potential for silicon[J]. Calphad-Computer Coupling of Phase Diagrams and Thermochemistry, vol. 31, pp. 95-104, 2007.

[33] S. Plimpton. Fast Parallel Algorithms for Short-Range Molecular-Dynamics[J]. Journal of Computational Physics, vol. 117, pp. 1-19, 1995.

[34] W. G. Hoover. Canonical dynamics: Equilibrium phase-space distributions[J]. Physical Review A, vol. 31, pp. 1695-1697, 1985.

[35] M. Parrinello, and A. Rahman. Crystal Structure and Pair Potentials: A Molecular-Dynamics Study[J]. Physical Review Letters, vol. 45, pp. 1196-1199, 1980.

[36] S. Alexander. Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool[J]. Modelling and Simulation in Materials Science and Engineering, vol. 18, pp. 015012, 2010.

[37] Y. B. Gerbig, S. J. Stranick, D. J. Morris, M. D. Vaudin, and R. F. Cook. Effect of crystallographic orientation on phase transformations during indentation of silicon[J]. Journal of Materials Research, vol. 24, pp. 1172-1183, 2009.

[38] R. Perez, and P. Gumbsch. Directional anisotropy in the cleavage fracture of silicon[J]. Physical Review Letters, vol. 84, pp. 5347-5350, 2000.
[39] R. Perez, and P. Gumbsch. An Ab initio study of the cleavage anisotropy in silicon[J]. *Acta Materialia*, vol. 48, pp. 4517-4530, 2000.

[40] T. Cramer, A. Wanner, and P. Gumbsch. Energy dissipation and path instabilities in dynamic fracture of silicon single crystals[J]. *Physical Review Letters*, vol. 85, pp. 788-791, 2000.

[41] D. Sherman, and I. Be'ery. From crack deflection to lattice vibrations - macro to atomistic examination of dynamic cleavage fracture[J]. *Journal of the Mechanics and Physics of Solids*, vol. 52, pp. 1743-1761, 2004.

[42] W. S. Ko, and B. J. Lee. Origin of unrealistic blunting during atomistic fracture simulations based on MEAM potentials[J]. *Philosophical Magazine*, vol. 94, pp. 1745-1753, 2014.

[43] J. A. Kerr, CRC *Handbook of Chemistry and Physics 1999-2000*. 81st ed. 2000: Florida: CRC Press.