Nucleation of Twinning Dislocation Loop in Pt: A Computational Approach

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Abstract

Twinning plays a critical part in the plastic deformation of the materials and the strengthening mechanisms and is hence considered as one of the most prevalent deformation mechanisms in metals. Because to the high stacking fault energy of the fcc metals like Al, Pd, and Pt, the extended dislocations are believed to be energetically favored over isolated partials, thereby rendering deformation twinning unfeasible. Nevertheless, some recent experimental researches have confirmed a potential deformation twinning pathway in nanocrystalline platinum. This alternate-shear mechanism has a much lower energy barrier than the usual layer-by-layer twinning. We utilize computations involving atomistic calculations and continuum modeling in this study to examine the genesis of deformation twins in Pt. Atomistic simulations provides the generalized planer fault energy using an EAM (embedded-atom-model) potential. Moreover, a potential energy-based method, namely; a nudged-elastic band (chain of states) has been used to compute the activation energy barrier for the nucleation of the twinning dislocation loop in the alternate-shear model. The critical stress needed for the nucleation of the twinning dislocation loop in platinum is estimated using some of the parameters acquired from atomistic calculations and using them as fitting parameters in the continuum model. The minimum-energy path between the two end states can be identified using this methodology. Through the unusual alternate-shear approach, the results provide a rudimentary but essential dislocation-based perspective of the occurrence of deformation twins in fcc metals.

Keywords: *Twinning; Atomistic simulations; Dislocation nucleation; Nudged-elastic-band*

1. Introduction

Under specific conditions, the plasticity of fcc metals and alloys are notably dictated by the process of deformation twinning. It is generally agreed upon that the stress needed for the evolution of deformation twins is mainly regulated by the metal's stacking-fault energy (SFE). In various studies, it has been found that the SFE of metals has to be low enough to show deformation twinning [1]. Investigations carried out experimentally on large-grained fcc metals, like copper and aluminum show no evidence of deformation twinning under normal conditions. Due to the high stacking fault energy, it is believed that the formation and glide of an extended dislocation are energetically favored over a twinning partial in the fcc metals like Al, Pd, and Pt [1,2]. This suggests that in such materials, the deformation twinning takes place only after adequate strain hardening has occurred to create high-stress concentrations. Strain hardening can be

accomplished by deformation conditions where recovery is suppressed, requiring either a very low deformation temperature or a high strain rate [3]. Though, once the grain size is reduced up to the sub-micron level, twinning can become a prominent mechanism of deformation in fcc metals, which is observed at normal room temperature and moderate strain rates. For fcc metals, a twin is nucleated by the layer-by-layer movement of partial dislocations, through the pole mechanism, prismatic gliding, faulted dipoles, and other mechanisms on consecutive, close-packed atomic planes [4]. But, only the shear model is feasible for nanocrystalline materials because of the availability of less space within a nanosized grain. Recent experimental studies administer imperative information on a novel route of deformation twinning in a nanocrystalline fcc material with very high stacking fault energy i.e., platinum [2]. The energy barrier for this proposed twinning pathway is substantially lower than that for conventional layer-by-layer twinning.

Platinum is a substantially important material for technological applications and Pt nanocrystals have attracted growing interest over the past decade. It is used broadly inside the present-day chemical and vehicle enterprise due to its high strength, excellent workability, and stability [5]. While the effects of twins on mechanical properties have been extensively investigated for metallic materials over the last decade, to the best of our knowledge, a detailed analysis of the twining pathways in the nanocrystalline Pt structure is still lacking, and investigations into this new twining pathway can provide a new and better understanding of the development of commonly observed deformation twins in it. Twinning is more complicated than slip: integrating shear, shuffles, and generation of new grain boundaries reminiscent of dynamic recrystallization. In this research, we exploit computations involving atomistic calculations and continuum modelling to picture the process of the formation of twining dislocation loops in NC Pt on the atomic scale. The energy pathways related with twinning involve the energy barriers which twinning partials must overcome while undergoing twin nucleation. We utilize atomistic simulations to calculate the generalized planer fault energy using an EAM potential. We perform a chain of state based nudged-elastic-band calculations, in order to find the minimum energy paths and the activation energy associated with the nucleation of the twinning dislocation loops and also to obtain the critical twinning stress. In this paper, the twin-energy pathways are integrated into a dislocation-based mechanistic model to envisage the same. It is expected to make a critical contribution in understanding the role of atomic structure and practiced stress in the nucleation event of twinning dislocation loops.

2. Modelling and Simulation

In nanocrystalline fcc materials, capturing the entire cycle of twinning dislocation nucleation is tricky and involves several steps. To determine the twinning stress, we consider the homogeneous nucleation of a twinning dislocation loop under various shear loads. The guide to speculating the twinning mechanism is the layer-by-layer accumulation of stacking faults which depends on the unstable twin fault energy (γ_{utf}) and thus makes twinning highly unfavourable in fcc metals with elevated γ_{utf} [2]. A new path of twinning has been observed experimentally which provides compelling evidence for the same in platinum which has very high $\gamma_{utf.}$ In layer-by-layer twinning, we have a slip of atomic plane along $11\bar{2}$ direction by an amount of a $<11\bar{2}>/6$. The slip occurs successively on the A plane, B plane, and C plane and hence it is also termed as ABC shear. But in an alternate shear mechanism also called ACB shear, the second slip occurs on the C plane after first slip on a plane which results in two adjacent layer of stacking fault. The final slip occurs on the B plane between these two stacking faults and creates a stable twin fault (Fig. 2).

2.1 Atomistic Simulation

The shear stress is applied on {111} atomic plane in $11\bar{2}$ direction. An atomistic simulation scheme that involves the method of chain-of states is used to compute the energy barrier for this nucleation process followed by the employment of a continuum analytical model, as stated by Aubry et al. [6]. The atomistic calculations performed here employed the parallel molecular dynamics code, LAMMPS [7], which is public-domain computer software developed at Sandia National Laboratory. The post-processing analysis and relevant calculation out of simulation data and the visualization is carried out with the OVITO program [8]. Common neighbour analysis (CNA) is used to image the defects. The red colour represents the hexagonal close-packed (hcp) atoms (corresponding to stacking faults and Twin boundaries), green represents perfect fcc atoms, and white indicates defected atoms. MATLAB is used as the post processing tool for data analysis, and theoretical validation.

To carry out atomistically informed nucleation modelling of the dislocation loop, a crystalline sample of Pt is constructed. The reciprocity between Pt atoms is described using an EAM potential, which is specified for Pt [9]. The choice of interatomic potentials is made by comparing its predictions with those of the DFT calculation results available in the literature, which accurately reproduces many of the material properties, including the fault energies that is relevant for simulations involving deformation. Also, the choice of interatomic potential plays an important role in the accuracy of the predicted energy barrier. The first part of atomistic computations uses the Climbing Image Nudged Elastic Band (CI-NEB) method [10] to estimate the minimum-energy paths of the nucleation of twinning dislocation loops. NEB is a generalized numerical algorithm that calculates path of minimum energy (MEP) between two stable atomic configurations [11]. The initial and final states are linked via a chain of multiple images or replicas of the system.

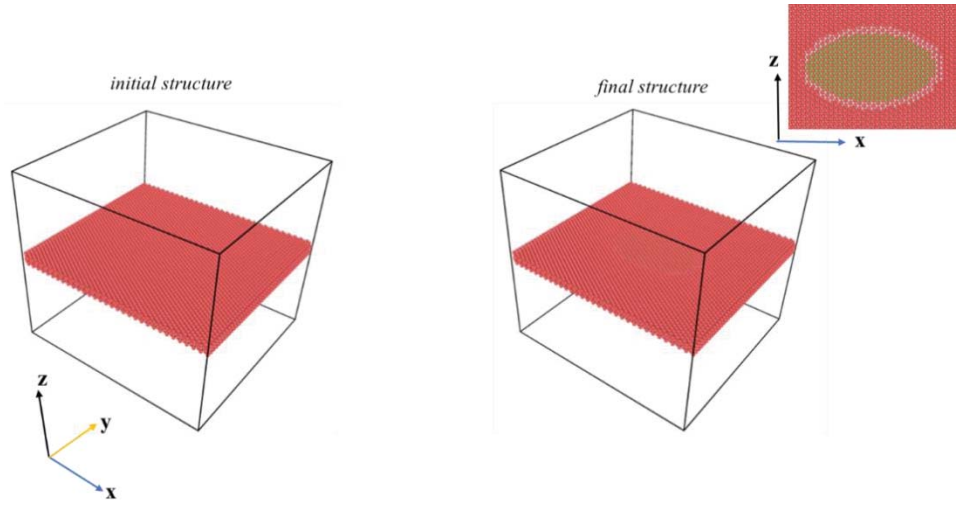

FIG 1. Typical structures of initial and final states for MEP search

The images unfold during the NEB computation in such a way that individual images find the state of lowest possible energy while conserving the equal spacing and eventually the chain lies along the path of minimum

energy. The initial state's simulation cell is composed of 184320 atoms in a fcc crystal of dimensions 16<11$\bar{2}$>×24<-110>×20<111>, with the x and z directions lying along the Burgers vector and the normal to the slip plane, respectively. Also, the crystal contains two adjacent intrinsic stacking faults with two twin boundaries as shown in Figure 1. The system is then relaxed and brought to the desired shear stress. The final state consists of a small dislocation loop set on the {111} slip plane between these two stacking faults as shown in Figure 1. The zoomed view is also shown adjacent to it.

The radius of the loop is chosen such that it expands spontaneously under the given stress range. In the entire three periodic boundary conditions (PBC) are imposed. Atomsk [12] is used for obtaining the final configuration of the crystal containing a dislocation loop. It is ensured that the energy of the final structure i.e., one containing loop must be less than the energy of the initial structure so that it doesn't fall into a metastable state. Using 16 replicas to discretize the path, the minimum energy paths (MEPs) have been determined. An energy tolerance of 1×10^{-10} eV together with the inter-replica spring constants of 5 eV Å−2 (k1) and 1 eV Å−2 (k2) is used to match the formerly employed tolerance. A large number of images enable a smooth activation energy map to be obtained. The results are seen and analysed using a visualization tool OVITO.

The second part involves the quantification of the GPFE, which is an important input parameter in the nucleation model as discussed in the next section. For the implementation of a continuum analytical model, as reported by Aubry et al. [6]. The GPFE is obtained by incrementally shifting the upper half crystal forth the direction of slip i.e. over the {111} atomic plane and calculating the difference in energies per unit area.

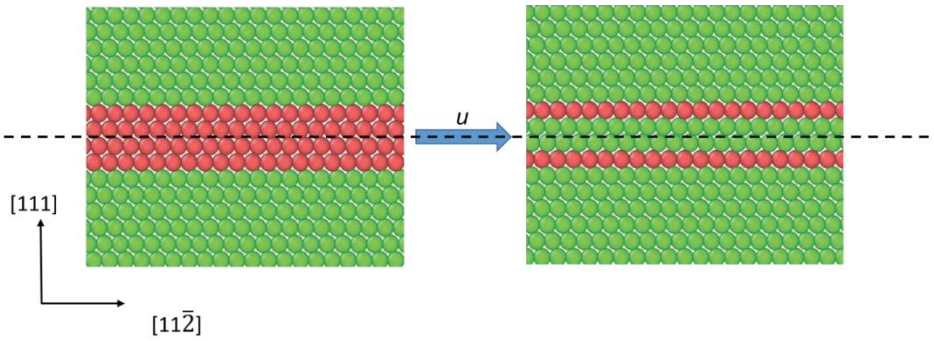

FIG 2. Schematic illustration of the new twinning route where the two SFs are present, a slip of a<11$\bar{2}$>/6 above the {111} slip plane results in formation of a two-layer twin-embryo.

The calculation of GPFE involves the change in the potential energy of the system or crystal as a function of the lateral shift. The initial structure is identical to that used for NEB computations, but with free surfaces normal to the <111> direction. At every single step of displacement in the lateral direction, the system is structurally relaxed so that the atoms move only normal to the plane undergoing slip. For the various values of stress, the GPFE is calculated using the below-mentioned equation

$$\gamma_{gpf}(u) = U(u) - U_i/A \quad \ldots (1)$$

Where, $U(u)$ stands for the total energy of the cell with the lateral displacement-vector u, U_i represents the energy of the lattice without any lateral displacement and A is the area of the faulted plane.

2.2 Continuum Modelling

To model the nucleation of a twinning dislocation loop in nanocrystalline fcc Pt under pure shear stress, we employ the method communicated by Aubry et al. [6], which calculates the energy required for the nucleation as a function of a stress-dependent GPFE and fractional Burgers vector b_f. The dislocation energy in the stated model is given as,

$$E(b_f, A; \sigma) = 2\pi r \frac{\mu b_f^2}{8\pi}\left[\frac{2-\nu}{1-\nu}\left(ln\frac{8R}{A} - 2\right) + \frac{1}{2}\right] + \left[\gamma_{gpf}(b_f + u_0; \sigma) - \gamma_{gpf}(u_0; \sigma)\right]A - b_f \sigma A \quad (2)$$

Most of the material parameters such as the effective elastic moduli, μ, and ν in the above equation are obtained from the EAM potential through the procedure described by Scattergood and Bacon [13]. Based on the available theories, it is difficult to determine the core radius. Therefore, it is used as a free parameter to fit the continuum model with the results generated from atomistic calculations at the average value of studied stresses. The saddle point at the specified stress in the 2-D landscape obtained from Eq. (2), gives the activation energy barrier. Using the appropriate μ, ν, and stress-dependent GPF energy allows us to match the results with the atomistic calculations.

3. Results and Discussions

In this work, we perform NEB calculation to study the new twinning pathway i.e. alternate shear mechanism in Pt at different stresses. The stress-dependent MEPs of the alternate shear model along with the climbing images (replica with the largest potential energy) visualized by the CNA method are shown in Figure 3.

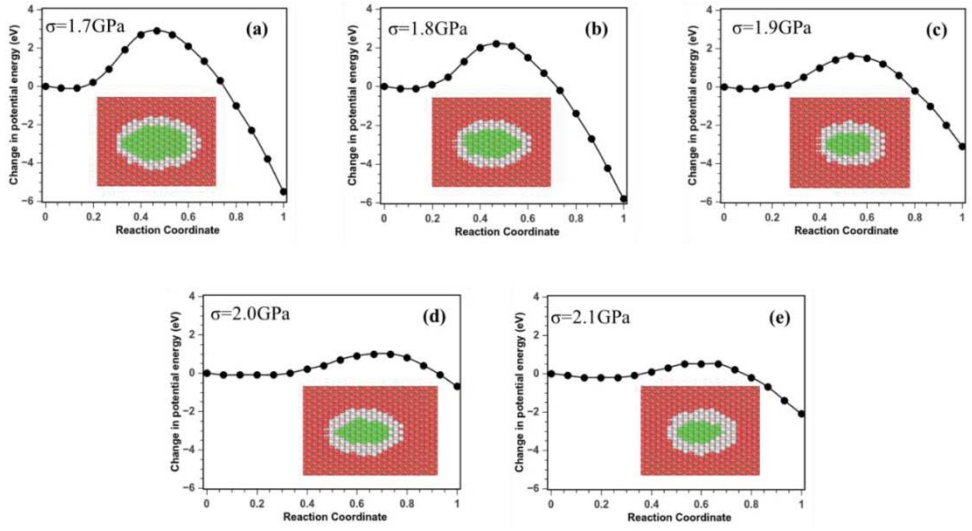

FIG 3. Plot for Minimum energy barrier for dislocation nucleation for A-C-B shear at different stress

The energy barrier is calculated at different stresses in range of 1.7 GPa to 2.1 GPa. The converged energy barrier varying with the application of applied stress is plotted in Figure 5(a), represented in filled squares. For the second set of calculations which involves the continuum modeling, the GPFE of Pt corresponding to our shear model is obtained. The calculation has been done for both the stressed and stress-free crystal. In this case the slip occurs on two alternate {111} planes, divided by a single plane between them. A third slip on this intermediate atomic layer creates the twin embryo. This process can be referred to as the A-C-B shear, where the generation of a partial dislocation between existing SFs induces twin nucleation. Figure 4 displays a curve representing the variation of generalized planer fault energy with the disregistry for both the stressed and stress-free crystals.

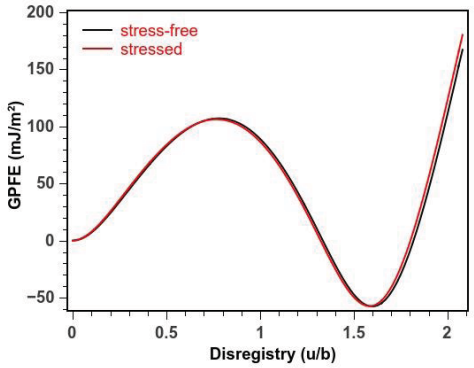

FIG 4. The GPF Energies for the stress-free and stressed crystals in the A-C-B shear mechanism.

We find a structure having some energy, which is lower than the initial energy of the structure, and conclusively represents negative stacking fault energy. By recognizing that the original structure with two stacking faults on alternate planes has increased structural energy, this uncommon behavior can be understood by the existence of four interceding hcp layers in between the fcc phase. A relative slip of $a\langle 11\bar{2}\rangle/6$ between the two neighboring stacking faults, as illustrated in Figure 2, let the two middle layers return to their face-centered cubic configurations. This gives a reason for the decrease in the energy of the system. Although the difference is very less, in the presence of an applied shear load, the displacements corresponding to the second minima in the GSFE profile get reduced below the original value of as evident from comparing Figure 4. Each pair of adjacent layers slides against each other due to the uniform shear strain caused by the stress applied. The figure shows that the applied shear stress also affects the GPFE profile. The declarations which are made from the atomistic data are correlated with those obtained from the continuum model and it shows a good concurrence between both of them (Figure 5(a)). One other interesting finding that has been observed is that the loop radius varies uniformly with the applied load. The trend is shown in Figure 5(b), where it displays that with an increase in the applied shear stress the loop radius is decreasing.

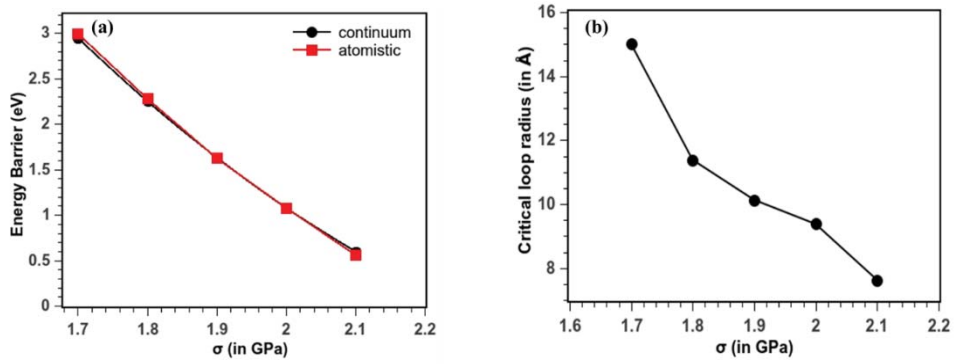

FIG 5. (a) E_a for dislocation nucleation as a function of applied shear stress for Pt in A-C-B shear. (b) Variation of the radius of the dislocation loop with applied stress

4. Conclusion

This study investigates the nucleation of twinning dislocation loops through the alternate shear mechanism in nanocrystalline Pt by utilizing a direct MEP-search technique and an atomistically informed continuum model. The continuum model has been shown to produce excellent fits to the results of the nudged elastic band measurements when tuned with a single free parameter. We report an unimpaired atomic-scale observation of this novel twinning route in NC Pt and these findings explain the broadly observed instances of deformation twins in fcc NC Pt despite its considerably high twinning energy barrier. This study thus offers an atomic-level understanding of the plastic deformation behaviour of FCC NC Pt.

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REFERENCES

[1] Zhao, X., Lu, C., Tieu, A.K., Zhan, L., Huang, M., Su, L., Pei, L. and Zhang, L., *Computational Materials Science*, *142*, 59-71 (2018).

[2] Wang, L., Guan, P., Teng, J., Liu, P., Chen, D., Xie, W., Kong, D., Zhang, S., Zhu, T., Zhang, Z. and Ma, E., *Nature communications*, *8*(1), 1-7 (2017).

[3] Yamakov, V., Wolf, D., Phillpot, S.R. and Gleiter, H., *Acta Materialia*, *50*(20), 5005-5020 (2002).

[4] Chowdhury, P. and Sehitoglu, H., *Journal of Engineering Materials and Technology*, *140*(2) (2018).

[5] Jeyaraj, M., Gurunathan, S., Qasim, M., Kang, M.H. and Kim, J.H., *Nanomaterials*, *9*(12), 1719 (2019).

[6] Aubry, S., Kang, K., Ryu, S. and Cai, W., *Scripta Materialia*, *64*(11), 1043-1046 (2011).

[7] Plimpton, S., *Journal of computational physics*, *117*(1), 1-19 (1995).

[8] Stukowski, A., *Modelling and Simulation in Materials Science and Engineering*, *18*(1), 015012 (2009).

[9] Zhou, X.W., Johnson, R.A. and Wadley, H.N.G., *Physical Review B*, *69*(14), 144113 (2004).

[10] Henkelman, G., Uberuaga, B.P. and Jónsson, H., *The Journal of chemical physics*, *113*(22),.9901-9904 (2000).

[11] Henkelman, G., & Jónsson, H., The Journal of chemical physics, 113(22), 9978-9985 (2000).

[12] Hirel, P., *Computer Physics Communications*, *197*, 212-219 (2015).

[13] Kauffmann, A., Freudenberger, J., Geissler, D., Yin, S., Schillinger, W., Sarma, V.S., Bahmanpour, H., Scattergood, R., Khoshkhoo, M.S., Wendrock, H. and Koch, C.C., *Acta Materialia*, *59*(20), 7816-7823 (2011).