# MECHANICS OF INTERACTION OF GROWING CRACK WITH GRAIN BOUNDARY IN BI-CRYSTAL SOLIDS

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**Abstract**
Molecular Dynamics (MD) simulations have been carried out to understand the mechanics of crack interaction with Grain Boundary (GB) under different scenarios. Specifically, different stages of a growing crack, like crack growth initiation and arrest at GB have been studied. The study was done by evaluating the Stress Intensity Factor (SIF) using near-tip stress field at each of these stages i.e. crack growth initiation and arrest at GB. To perform this simulation, an understanding of rotation transformation has been applied to form an aluminum bi-crystal.

## 1. Introduction

Grain boundary (GB) plays a vital role in the crack propagation of a material. The effect of GB can be easily understood when the material studied is a bi-crystal. A GB can completely arrest a propagating crack, arrest for some time and/or change the direction of crack propagation. Not only the GB, but also the orientation of the crystal on the other side of the GB, together determine the fate of the crack. Crack can easily propagate along the weak plane of the crystal. However, when the crack is not aligned along the weak plane (for example on the other side of the GB), crack propagation behavior changes, which needs to be studied in detail. While studying such problems on atomistic scale using Molecular Dynamics (MD) simulation, formation of bi-crystal was found to be a challenging task. Some software provides an easy method to form such a structure, but it is not convenient for all structures. Hence, proposing a generalized method for developing bi-crystals was needed. In this work, the mechanics of crack initiation and arrest at GB has been studied by evaluating SIFs using the near tip stress fields.

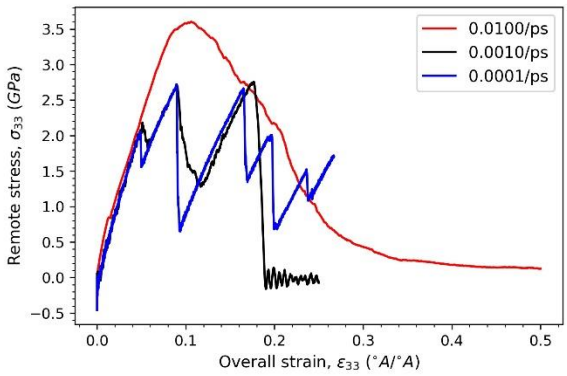
## 2. Results

MD simulations were performed after the formation of bi-crystal and analyses were performed to understand the role of different GBs in crack propagation of bi-crystal aluminum. Dimension of the structre is $243$ nm $\times$ $81$ nm $\times$ $162$ nm. Crack length is $60\ nm$. Total number of atoms used is 195000. Boundary condition are periodic along the thickness direction (<010>) and non-periodic along other two direction. Simulation is performed with NPT condition and <001> is the pulling direction. The following are important steps of this study.

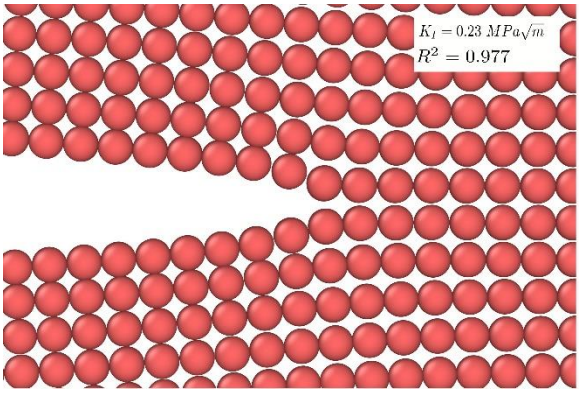
a. Bi-crystals are formed by joining crystals of different orientations at the GB. Each crystal of different orientation is prepared by rotating the single crystal oriented along <100>, <010> and <001>. The rotation matrix for the this transformation about the rotation axis $\hat{n}$ for an angle $\theta$ is $R(\theta) = nn^T + cos\theta(1 - nn^T) + sin\theta S(n)$, where $S(n)$ is a skew symmetric matrix dependent on the coefficients of $\hat{n}$. In present case, $\hat{n}$=<010> and $\theta = 30°$.
b. Two important stages of fracture; crack growth initiation and arrest have been observed and their SIF have been calculated using near-tip stress field. Validity of this method is justified from the fitting parameter $R^2$, while fitting the virial stress $\sigma_{33}$ vs $1/\sqrt{2\pi r}$, where $r$ is the distance ahead of the crack tip. When $R^2$ value is quite close to 1, linear elasticity is assumed to be valid. If it's quite less, then linear elasticity cannot be assumed to be valid in the near-tip region.

In Fig. 1a, the stress-strain variation for three different strain rates has been presented. It can be observed that, for strain rate of 0.001/ps and 0.0001/ps, the nature of stress-strain curve is similar. However, for 0.01/ps it is different from former two and its peak stress is also expectingly higher. Hence, the lower strain rates can be assumed to resemble quasi-static behavior. Two important stages of a growing crack have been shown in Fig. 1, where important stages like crack growth initiation (Fig. 1b) and arrest at GB (Fig. 1c)

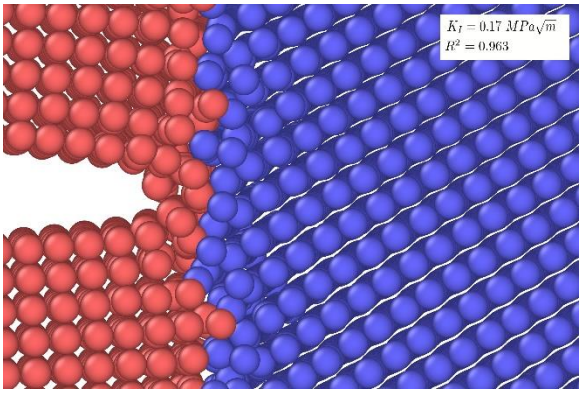
have been shown with the value of SIFs along the crack direction. Their SIFs are shown in Fig. 1d with the respective $R^2$ values shown in adjacent brackets to dots. In Fig. 1d , the SIFs at the crack initiation have been shown in black dots and SIFs for arrested crack at the GB have been shown in red dots. As per values of SIFs and respective $R^2$, the linear elasticity approximation is valid in the left crystal. Later, when the growing crack reaches the GB, it is gets arrested and started blunting.



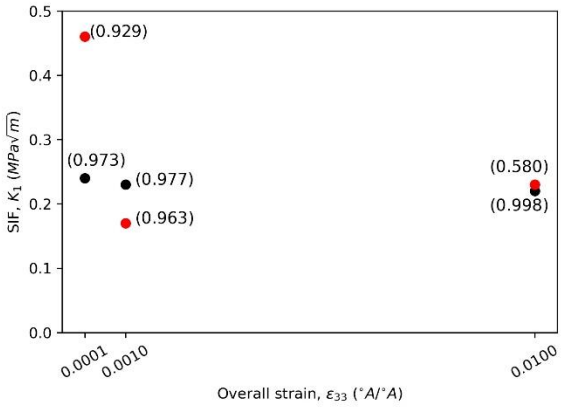

a) Remote stress-strain for different strain rates




b) Crack growth initiation at $\epsilon_{33} = 0.050$




c) Crack growth arrest at GB at $\epsilon_{33} = 0.056$




d) SIFs at crack growth initiation and arrest

Fig. 1 – Different stages of crack propagation showing crack initiation and arrest at GB with SIFs

By looking at the $R^2$ values of arrest, it can be said that at the initial stage of crack arrest, linear elasticity is valid with quasi-static strain rates only. It may be also observed that the crack growth initiation SIF for all strain rates is almost the same with over 97% $R^2$ suggesting the validity of linear elasticity at this stage.

## 3. Conclusions

In this study, a unique method of creating a general bi-crystal for MD simulation has been used. The role of GB in crack propagation has been explained. Linear elasticity has been found to be valid during crack growth initiation for all strain rates and for arrest at GB it is valid only with slower quasi-static strain rates. Influence of strain rate on the crack propagation has been studied. It has been found that at a low strain rate, crack could grow further in the crystal ahead of the GB with a little blunting. However, at an extremely slow loading rate, crack could not propagate further from GB; instead, the crack tip got blunted at the GB.