

## Accepted Manuscript

Molecular dynamics modeling of crack propagation in titanium alloys by using an experiment-based Monte Carlo model

Xiangguo Zeng, Tixin Han, Yang Guo, Fang Wang

PII: S0013-7944(17)30893-7  
DOI: <https://doi.org/10.1016/j.engfracmech.2017.12.012>  
Reference: EFM 5793

To appear in: *Engineering Fracture Mechanics*

Received Date: 27 August 2017  
Revised Date: 26 November 2017  
Accepted Date: 8 December 2017

Please cite this article as: Zeng, X., Han, T., Guo, Y., Wang, F., Molecular dynamics modeling of crack propagation in titanium alloys by using an experiment-based Monte Carlo model, *Engineering Fracture Mechanics* (2017), doi: <https://doi.org/10.1016/j.engfracmech.2017.12.012>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Molecular dynamics modeling of crack propagation in titanium alloys by using an experiment-based Monte Carlo model

Xiangguo Zeng<sup>a</sup>, Tixin Han<sup>a</sup>, Yang Guo<sup>a</sup>, Fang Wang<sup>b,\*</sup>

<sup>a</sup> *College of Architecture and Environment, Sichuan University, Chengdu, Sichuan 610065, China*

<sup>b</sup> *Faculty of Materials and Energy, Southwest University, Chongqing, 400715, China*

**Abstract:** Based on extensive experiments at the microscopic level, it was found that the grain sizes of TA1 titanium alloys exhibited a statistical nature, and in turn, the resultant distribution was achieved by a data fit. The Monte-Carlo method was employed to obtain a model size for molecular dynamics simulations. The melting point and lattice constants of the alloys were calculated using LAMMPS software with the model dimension. A comparison of numerical results and published experimental results was presented to demonstrate that such a method provides a reasonable domain that is beneficial to molecular dynamics modeling. Afterwards, a cohesive element model along the effective simulation region was established, and

---

*Abbreviations:* MD, molecular dynamics; CZM, cohesive zone model; 2D, two dimensional; T-S: traction-separation.

\* Corresponding author. Tel: +86-23-68253204; fax: +86-23-68254373.

*E-mail address:* wangfang\_cq1978@163.com (F. Wang)

Download English Version:

<https://daneshyari.com/en/article/7169069>

Download Persian Version:

<https://daneshyari.com/article/7169069>

[Daneshyari.com](https://daneshyari.com)