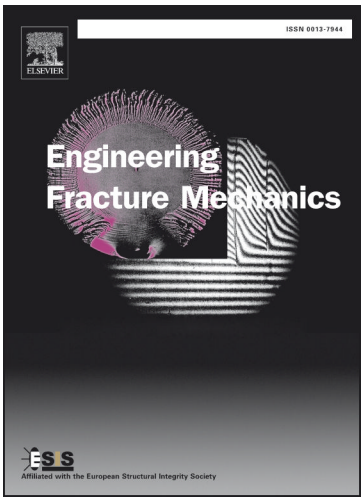

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Molecular dynamics modeling of crack propagation in titanium alloys by using an experiment-based Monte Carlo model

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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.

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