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Central-force decomposition of the tersoff potential

The Hung Tran, author

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Abstrak

ABSTRAK

Central forces play important role in the analysis of results obtained with particle simulation methods, since they allow evaluating stress fields. In this work we derive expressions for a central force decomposition of the Tersoff potential, which is often used to describe interatomic interactions in covalently bonded materials. We simplify the obtained expressions and discuss their properties.