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Quasilattice-conserved molecular dynamics study of the atomic structure of decagonal Al-Co-Ni quasicrystals YU-JUN ZHAO, XIAOTIAN LI, South China University of Technology, ADVISOR-STUDENT COLLABORATION — The detailed atomic structure of quasicrystals has been an open question for decades. In this paper, we present a quasilattice-conserved molecular dynamics method (quasiMD), with particular quasiperiodic boundary conditions. As the atomic coordinates are described by basic cells and quasilattices, we are able to maintain the self-similarity characteristics of qusicrystals with the atomic structure of the boundary region updated timely following the relaxing region. Exemplified with the study of decagonal Al-Co-Ni (d-Al-Co-Ni), we propose a more stable atomic structure model based on Penrose quasilattice and our quasiMD simulations. In particular, "rectangle-triangle" rules are suggested for the local atomic structures of d-Al-Co-Ni quasicrystals.

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