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Internal friction of grain boundaries in two-dimensional Yukawa solids

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Langevin dynamics simulations are performed to investigate the grain boundary internal friction (GBIF) in two-dimensional (2D) Yukawa solids under oscillating shear deformations. It is discovered that the GBIF exhibits a significant transition with the increasing misorientation angle, which can be used to distinguish the low- and high-angle grain boundaries (GBs) [1]. From the dependence of the GBIF on the shear amplitude and frequency, it is found that the internal friction of high-angle GBs exhibits typical properties of the linear anelasticity, corresponding to the typical anelastic properties [2]. However, the GBIF of low-angle GBs does not. The variation trend of the calculated GB stiffness with the misorientation angle well agrees with that of GBIF, while the GB stiffnesses of the low- and high-angle GBs are both independent of frequency. For the transition between the low- and high-angle GBs of the misorientation angle $\theta = \pi/9$, the corresponding GB migration exhibits the normal diffusion, completely different from the ballistic motion of the GB migration of other misorientation angles.

Our obtained the GBIF Q^{-1} of a 2D Yukawa solid are presented in Figure. 1. We discover that the obtained GBIF exhibits a prominent transition around the misorientation angle between $\pi/9$ and $5\pi/36$, corresponding to the transition of the GB from the low-angle GB to the high-angle GB. From our understanding, the difference in geometric structure between the low- and high-angle GBs leads to the fundamental change of the GBIF. The low-angle GBs are composed of discrete dislocations, so that the interaction between these dislocations is much weak. While in the high-angle GBs, the composed dislocations are connected together, just corresponding to the strong coupling.

References
[1] S. Lu, D. Huang, C. Liang, and Yan Feng, Phys. Rev. B 111, 174112 (2025).
[2] S. Lu, D. Huang, C. Liang, and Yan Feng, Phys. Rev. Research 5, 043116 (2023).

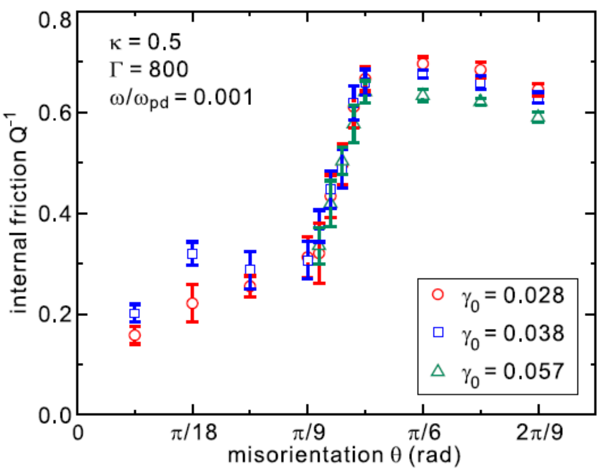

Figure. 1. Obtained GBIF Q^{-1} of 2D Yukawa solids as both the misorientation angle θ and the shear strain amplitude vary. When the misorientation angle θ increases gradually from $\pi/36$ to $2\pi/9$, Q^{-1} clearly exhibits a transition between $\pi/9$ and $5\pi/36$, which divides the GBs into two groups, just corresponding to the low- and high-angle GBs, respectively. For the low-angle GBs of $\theta < \pi/9$, the value of Q^{-1} increases slightly with θ. For the transition of $\pi/9 < \theta < 5\pi/36$, the value of Q^{-1} increases sharply with θ. While, for the high-angle GBs of $5\pi/36 > \theta$, the value of Q^{-1} is always around 0.65.