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Orientation dependences of surface morphologies and energies of iron-gallium alloys[1] MARCIO COSTA, HUI WANG, JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, SUOK-MIN NA, HYUNSUK CHUN, ALISON B FLATAU, Department of Aerospace Engineering,?University of Maryland, College Park, MD , UNIVERSITY OF CALIFORNIA, IRVINE COLLABORATION, ?UNIVERSITY OF MARYLAND COLLABORATION — Magnetostrictive Fe-Ga alloys (Galfenol) are very promising rare-earth free materials for applications in sensors, actuators, energy-harvesters and spintronic devices. Investigation on surface energies of Galfenol based on density functional calculations (DFT) and contact angle measurements may provide fundamental understandings and guidance to further optimize the performance of Galfenol. DFT calculations predict that Ga-covered (110) surface of Galfenol is more stable in Ga-rich condition, while Ga-covered (001) surface of Galfenol surface become more favorable in Ga-poor condition. Moreover, a full Ga overlayer tends to form on top of Gafenol surfaces regardless their orientation, both in agreement with the experimental observation. Further studies on Ga segregation in the Fe bcc matrix demonstrate that the Fe-Ga separation is unlikely to occur since Ga diffusion toward the surface is effectively self-stopped once the Ga overlayers form on the facets.

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