



Contributions of atomistic simulations to the understanding of the formation and evolution of defects in crystalline materials

Julien Guénolé

► To cite this version:

Julien Guénolé. Contributions of atomistic simulations to the understanding of the formation and evolution of defects in crystalline materials. Invited Lecture at Beijing Jiaotong University, Jun 2021, Online, China. hal-03388532

HAL Id: hal-03388532

<https://hal.univ-lorraine.fr/hal-03388532>

Submitted on 20 Oct 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Contributions of atomistic simulations to the understanding of the formation and evolution of defects in crystalline materials

Dr. Julien GUÉNOLÉ^{1,2}

¹ CNRS, Université de Lorraine, LEM3, Metz, France

² LabEx DAMAS, Université de Lorraine, Metz, France

julien.guenole@univ-lorraine.fr

To tackle the scientific and industrial challenges ahead, the availability of novel high-performance materials will be of prime importance. To this aim, modern laboratories and industries heavily rely on models and numerical simulations to foster the design of tailored properties materials. In this context, atomistic modelling provides a unique access to fundamental material mechanisms able to support innovative physics-based constitutive models for material design.

Here we present the contribution of atomistic simulations towards the development of higher-scale models, though the understanding of the plastic deformation of crystalline materials. The Molecular Dynamics method will be presented and compared with other approaches, such as Density Functional Theory approaches and Monte Carlo simulations. Then, examples of investigations will be presented and discussed. The dislocation absorption in GBs and the influence of internal strain on irradiation-induced damage will be shown as examples of inputs in higher scale models¹. The interplay of atomistic simulations and experiments will be highlighted through the investigation of irradiation damage², the formation of defects in MAX phases^{3,4}, the initiation of plasticity in nanowires^{5,6}, and the dislocation-interface interactions in metallic composites^{7,8} and superalloys⁹. The focus of this lecture will be the inputs provided by these atomistic simulations to higher scale techniques and the interplay with experiments.

References

1. Korsunsky, A. M. *et al.* Quantifying eigenstrain distributions induced by focused ion beam damage in silicon. *Mater. Lett.* **185**, 47–49 (2016).
2. Chang, Y. *et al.* Ti and its alloys as examples of cryogenic focused ion beam milling of environmentally-sensitive materials. *Nat. Commun.* **10**, 942 (2019).
3. Yu, W., Guénolé, J., Ghanbaja, J., Vallet, M. & Guitton, A. Frank partial dislocation in Ti2AlC-MAX phase induced by matrix-Cu diffusion. *Scr. Mater.* **191**, 34–39 (2021).
4. Guénolé, J., Taupin, V., Vallet, M., Yu, W. & Guitton, A. *Features of a nano-twist phase in the nanolayered Ti3AlC2*. <https://hal.univ-lorraine.fr/hal-03207521> (2021).
5. Guénolé, J., Godet, J. & Brochard, S. Plasticity in crystalline-amorphous core-shell Si nanowires controlled by native interface defects. *Phys. Rev. B - Condens. Matter Mater. Phys.* **87**, 1–10 (2013).
6. Lee, S. *et al.* In-situ observation of the initiation of plasticity by nucleation of prismatic dislocation loops. *Nat. Commun.* **11**, 1–11 (2020).
7. Vaid, A., Guénolé, J., Prakash, A., Korte-Kerzel, S. & Bitzek, E. Atomistic simulations of basal dislocations in Mg interacting with Mg17Al12 precipitates. *Materialia* **7**, 100355 (2019).
8. Guénolé, J. *et al.* Exploring the transfer of plasticity across Laves phase interfaces in a dual phase magnesium alloy. *Mater. Des.* **202**, 109572 (2021).
9. Prakash, A. *et al.* Atom probe informed simulations of dislocation-precipitate interactions reveal the importance of local interface curvature. *Acta Mater.* **92**, 33–45 (2015).