General theory of the Kanzaki force field applied to extended defects

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ABSTRACT

Kanzaki forces[1] are a standard way of representing point defects in the elastic continuum. They are the forces that would have to be applied on a perfect, defect-free crystalline lattice to generate the topology of the point defect. By computing these forces in atomistic lattices, one obtains a true multiscale representation of the point defect.

In this talk, I generalise the concept of Kanzaki force to all other crystalline defects. I will discuss how the resulting Kanzaki force fields are to be computed for any general defect, including dislocations, grain and twin boundaries, or cracks. This enables an accurate representation of the atomistic topology of extended defect in the elastic continuum, and a rigorous multiscale transfer of information from the atomistic lattices to the elastic continuum.

I will focus on obtaining the Kanzaki force field of crystallographic dislocations, both edge and screw [2]. I will show that the Kanzaki force field of a dislocation consists of two separate components: a Volterra contribution associated with the disregistry that characterises the dislocation, and a core contribution associated with the specific topology of the dislocation core. I will then show how to use each of these components to model the dislocation core in the elastic continuum, and obtain an atomistically informed model of the dislocation. Unlike other regularisation procedures like the Peierls-Nabarro model, the resulting models are topologically true to the dislocation core, and energetically accurate up to the harmonic approximation.

Finally, I will discuss how the Kanzaki force field can be employed to study dislocation mobility using lattice dynamics[3], and I will highlight several lattice instabilities that arise when screw and edge dislocations, modelled using Kanzaki forces, are driven at high speeds.

REFERENCES

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[3] Verschueren, J., Gurrutxaga-Lerma, B., Balint, D. S., Sutton, A. P., & Dini, D. (2018). ‘Instabilities of high speed dislocations.’ *Phys. Rev. Lett.*, 121(14), 145502.