Final Project: Prediction of elastic response of a metal matrix composite

Goals

For the final project, your goal is to predict the elastic response of a hypothetical metal matrix composite (MMC) using computational tools. Your metal matrix will be aluminum, whose elastic constants you have already computed. The reinforcement will be tantalum carbide (TaC), which forms in the rocksalt ($Fm\bar{3}m$) structure. You will need to (a) compute the elastic constants for TaC from first principles, and (b) investigate the effect of spatial distribution and orientation on the elastic properties of this MMC.

Successful completion of this work will demonstrate competence in using both DFT and FEM software to analyze material elastic response, and the ability to design your own computational study.

Deliverables

You will produce a detailed (5–8) page report that includes an Abstract, Introduction, Methods, Results and Discussion, Conclusions, and Bibliography. This will be graded on your

1. design of computational materials research project (20%),
2. appropriate and competent use of computational tools (50%), and
3. clarity of the report (30%)

The report should be formatted as a single pdf document. Submit your **PDF file** via Assignment Upload by **11:59pm on 15 March 2018. Late submissions will not be accepted.**

1. Density functional theory calculation of TaC elastic constants

You will need to compute the elastic constants of TaC using `QuantumEspresso`. You should use the PAW potentials with the PBE exchange-correlation potential, with a scalar relativistic treatment. As with aluminum, you will need to (a) perform and demonstrate convergence with respect to computational parameters, (b) determine the relaxed structural parameters, and (c) compute the anisotropic elastic constants for TaC.

2. Finite element method calculation of Al-TaC MMC elastic response

You will investigate the effect of shape and orientation on the elastic response of a hypothetical MMC. A simple generalization of the volume fraction rule includes an empirical prefactor corresponding to geometric effects:

$$E_{\text{composite}} = E_{\text{matrix}}(1 - V_{\text{f}}) + \alpha E_{\text{reinforcement}} V_{\text{f}}$$

where V_f is the volume fraction of reinforcement, E_matrix and $E_\text{reinforcement}$ are the corresponding Young's moduli, and $0 < \alpha < 1$ is an empirical parameter that captures the geometric contributions. In `/class/mse404ela/FinalProject`, you will find four different "microstructures" corresponding to regular arrays of circular and rectangular reinforcements as well as random arrangements of the same. Use these images as your basis to study the effect of shape, arrangement, and orientation on the elastic response. As you did previously, you will need to (a) develop and critique your choice of skeleton, (b) determine elastic response, and (c) investigate the distribution of stress in your material.

Conclude your assessment with a recommendation of preferred reinforcement structure to optimize the elastic response based on your findings.