# A Concept of a Representative Atomic Volume for a Grain

A. Gubanov* and O. Vinogradov**

Department of Mechanical and Manufacturing Engineering,
Schulich School of Engineering, University of Calgary,
Calgary, Alberta, T2N 1N4, Canada
*artem.gubanov@gmail.com, **ovinogra@ucalgary.ca

## ABSTRACT

In the present work a concept of a Representative Atomic Volume (RAV) for a grain based on atomistic simulations is proposed. It is tested on a cubic $\alpha$ – iron polycrystal structure comprised of eight grains with different grain sizes. Considering as a criterion the Young's modulus, it is shown that the grain size comprising of twelve normalized units is sufficient to be considered as a RAV for a grain embedded in a polycrystal.

***Keywords***: representative atomic volume, grain size, polycrystal, molecular statics, atomistic simulation

## 1 INTRODUCTION

It is known that materials microstructure (defects, grains sizes, grain boundaries, etc.) defines its bulk properties. The challenge is to establish this relationship numerically through computer simulations. In spite of the fact that with the increasing computer power it became possible to conduct large scale atomistic simulations (of up to billion atoms) [1], it is still impossible to handle the number of atoms present in a sample on the true macro-scale level [2]. Instead, various multi-scale simulations approaches developed in recent years [2-4] address this challenge.

An alternative approach can be based on the concept commonly used in composite materials and other discrete systems, namely, on the so-called, representative volume element (RVE) [5, 6]. By definition, the RVE is the smallest discrete system of a composite material which correctly reflects the behaviour of the experimental specimen representing the continuum. In the case of atomistic simulations, such an element can be named a representative atomic volume (RAV) in order to distinguish it from the conventional RVE term since, as it will be clarified below, it involves convergence to continuum of two discrete system simultaneously, the atomistic, on a nanoscale, and the grains, on a mesoscale. To the best of our knowledge, such an element was never numerically established for any material. The numerical implementation of the concept of RAV in the case of atomic systems is not straightforward. The direct application of the concept known in composite materials would assume numerical experiments with single grain (crystal) having different sizes and crystallographic orientations. However, such an approach would not take into account the effect of grain boundaries on this RAV. At the same time, as it well known [7], grain size and boundaries produce significant effect on bulk materials properties. The approach suggested in the present paper allows establishing the RAV of an ideal grain while taking into account the fact that this grain is interacting with other grains at their boundaries. This approach is implemented in the following way. A system of polycrystals with the same number of grains but having different grain sizes and crystallographic orientations is generated and tested numerically. The result of each numerical test is the stress-strain curve. When for a specific grain size the stress-strain curve does not change with the further increase of the grain size (for the same number of grains in a polycrystal) then this grain size characterises the RAV for a grain. This approach is tested in the present paper on the cubically shaped polycrystal comprising 8 grains of $\alpha$ – iron.

## 2 SIMULATION METHODOLOGY

There are three fundamental steps defining the results of molecular statics (MS) simulations of polycrystals composed of ideal grains: the polycrystal generation method, the loading method, and the relaxation procedure. The polycrystal generation procedure involves generation of a 3D system of grains with each having random size, shape and crystallographic orientation. In addition, the boundaries between the grains should be such that the distance between two atoms situated at the boundaries of two neighbouring grains does not exceed the equilibrium distance between these atoms. In other words, no additional atom can be inserted into grains boundaries without supplying additional energy.

A simple and efficient method of generating a polycrystal which reflects the topological properties of a real material is based on using a 3D Voronoi diagram decomposition procedure [8]. The details of this approach will be given in [9].

The system of atoms comprising the polycrystal is divided into three sets: two of them are associated with the specimen boundaries (these boundaries are subjected to incremental displacements in opposite directions along the x-axis) and the third one comprising of atoms between the

two boundaries. The latter one is subjected to relaxation after each loading step.

In this paper a modified method of minimization suggested in [10] has been utilized. This method is based on independent displacements of atoms and allows parallel computations and thus use of high performance computing system WestGrid [11] that is available for the research purposes at the University of Calgary. As it was shown previously [12, 13], the iterative method of energy minimization suggested in [10] allows obtaining any desired level of accuracy in terms of unbalanced forces between the atoms. The numerical results are given for the pairwise Morse potential, which is suitable for the $\alpha$ – iron with body-centered cubic (BCC) lattice cell [14].

Figure 1 illustrates a sample polycrystal comprising eight grains after initial relaxation procedure applied to the entire sample.

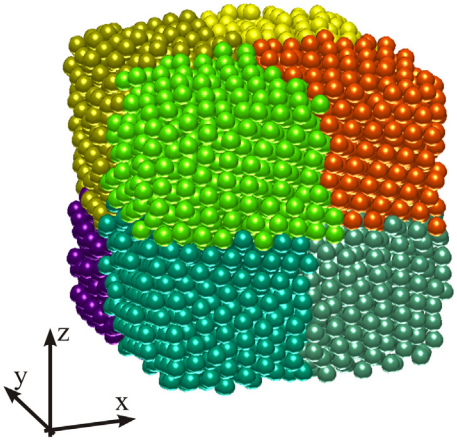


Figure 1: An example of a relaxed 8 grains polycrystal. Different colors represent different grains. The grain relevant size is seven normalized units and the total number of atoms is 4943.

Figure 2 shows engineering stress-strain curve for this sample. All interatomic distances are normalized by the lattice constant. The cutoff distance for defining neighbouring atoms was set to 2.55 normalized units. The convergence criterion for the maximum allowed unbalanced force was set to $0.001*10^{-9}$ N. The thickness of both boundaries is defined by a cutoff distance measured from the atoms layers of the sample surfaces. The step of loading was chosen to be 0.01 normalized units to assure smooth and sufficiently detailed stress-strain relationship.

Although a simple pairwise Morse potential used in the present study may distort the plastic part of the stress-strain curve, the elastic one, used in the present analysis, does reflect the properties of a single crystal [15, 16] and it justifies its use in the form of the Young's modulus as a criterion for the assessment of the RAV.

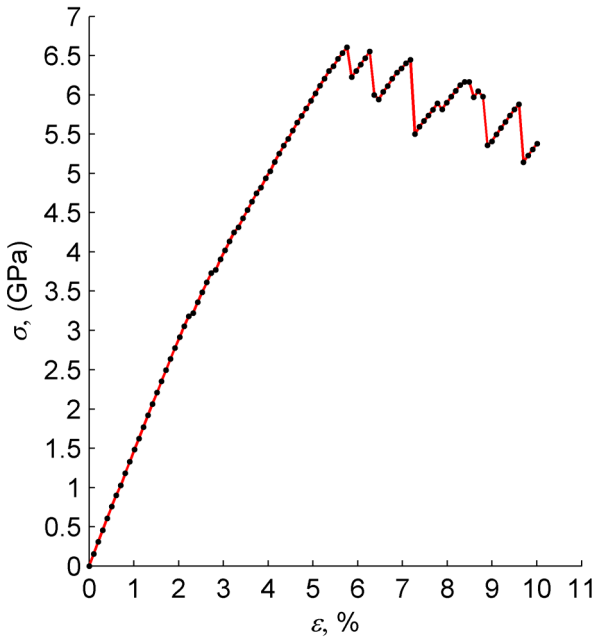


Figure 2: Engineering stress-strain curve. Simulation data is represented as black points which are connected by straight lines.

A snapshot of the polycrystal in Figure 1 after extension to a 10% strain is shown in Figure 3.

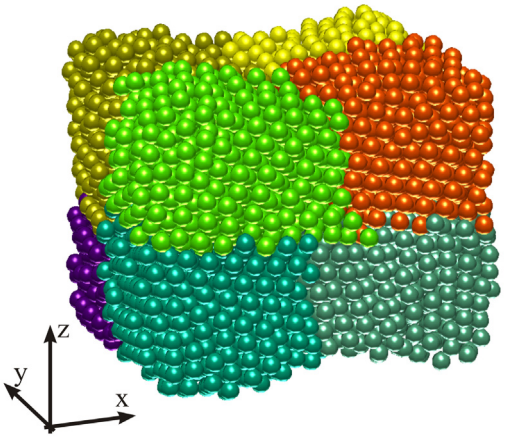


Figure 3: A polycrystal at the 10% strain.

## 3 RAV FOR A GRAIN

As it was mentioned above, the model must adequately reflect the reality. In this work the criterion for the RAV selection is the requirement that the Young's modulus of the sample does not change with further increase of the sample size. For defining a RAV for a grain embedded in a polycrystal, a symmetric structure comprised of eight

relevant same-size grains, 2 by 2 by 2, was considered and numerical experiments for different sample sizes, due to different sizes of grains, were conducted. In order to eliminate statistical fluctuations caused by the effects of grain boundaries and crystallographic orientations, 15 same-sizes (but varying in crystallographic orientations and grain shapes) samples were analyzed and then the ensemble average was calculated.

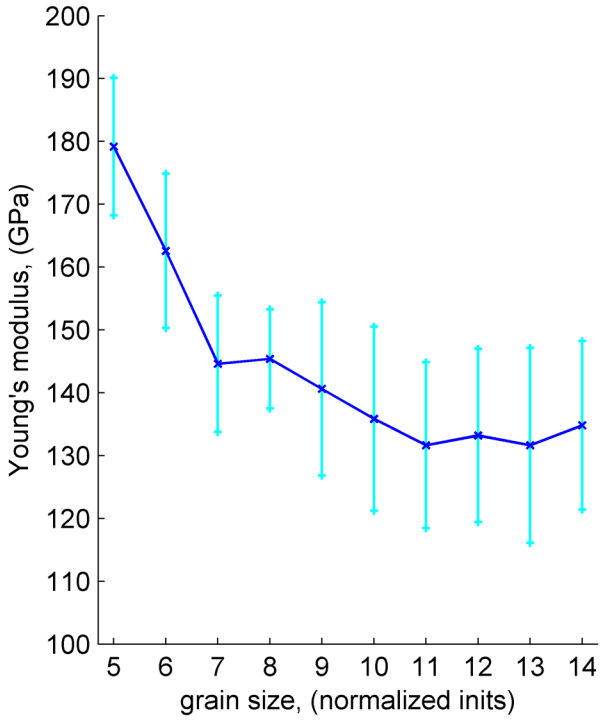


Figure 4: Average Young's modulus with standard deviation bars for 8 grains samples with different relevant grain sizes (grains have the same relevant size for every sample). For every grain size 15 samples were generated and tested.

Figure 4 illustrates the dependence of the Young's modulus on the sample's relevant grain size. The strain limit, to define the Young's modulus, was set to 2.5%, which was within the range of elastic deformations. It is seen that in this specific case the grain size comprising around 12 normalized units (about 3.4 nm, 3250 atoms) is sufficient to be considered as a RAV for a grain. For the smaller grain sizes the effect of crystallographic orientations and grain boundaries plays a more significant role in scattering the sample properties.

## 4 CONCLUSION

The concept of a representative volume for a grain embedded in a polycrystal is introduced and tested for an $\alpha-$iron BCC lattice cell. It is shown that such a RAV exists when various grains sizes, shapes, and random crystallographic orientations are taken into account. This is an important step in developing a RAV for a polycrystal in which the number of grains will be varied while each grain will have the minimum number of atoms found through RAV simulations in the first step (for a single embedded grain).

The RAV for a polycrystal is an alternative way of multiscale modeling. Such a RAV can be used to assess bulk properties of the materials while taking into account topological changes (such as dislocations formation, cracks initiation, etc) taking place on a nano-and meso-scale during deformations.

The results presented here justify further research on RAV for grains and polycrystals in which pre-existing point, line and surface defects are present.

## 5 ACKNOWLEDGEMENT

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