Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A GPU enhanced approach to identify atomic vacancies in solids materials[1] JOAQUIN PERALTA, CLAUDIA LOYOLA, Universidad Andres Bello, SERGIO DAVIS, Universidad de Chile — Identification of vacancies in atomic structures plays a crucial role in the characterization of a material, from structural to dynamical properties. In this work we introduce a computationally improved vacancy recognition technique, based in a previous developed algorithm. The procedure is based in the use of Graphics Processing Unit (GPU) instead of Central Processing Unit (CPU), taking advantage of random number generation as well the use of a large amount of simultaneous threads as available in GPU architecture, improving the spatial mapping in the sample and the speed during the identification process of atomic vacancies. The results show that with this technique, efficiency is improved. Along with the above a reduction of required parameters in comparison with the original algorithm is presented. We show that only the lattice constant and a tunable overlap are enough as input parameters in the process, and are also highly related. A study of those parameters is presented, suggesting how the parameter choice must be addressed. Benchmarks were made using one standard CPU and GPU between the original code and the present work, revealing an improvement in the execution time.

[1]This work is supported by FONDECYT Iniciacion 2013, 11130501

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Date submitted: 14 Nov 2014 Electronic form version 1.4