MAR05-2004-001524

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

**Accuracy of high throughput ab-initio methods in predicting crystal structures of metals: review of 80 binary alloys**

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Predicting and characterizing the crystal structure of new alloys is a key problem in materials research and development. It is typically addressed with either accurate *ab initio* calculations on a small set of candidate structures or with empirical rules that have been extracted from a large body of experimental information, but have uncertain predictive power. One inherent limitation of most *ab initio* approaches is that they do not make explicit use of results of previous calculations when studying a new system. In heuristic models, a large set of experimental observations is used to extract rules that rationalize crystal structure with a few simple physical parameters (e.g. atomic radii, electronegativities, etc.). An innovative and powerful tool to tackle the prediction problem is the high-throughput *ab initio* method, which makes use of robust automated techniques to perform many thousands of calculations. By creating a huge database of over 14,000 *ab initio* structural optimizations on a set of 80 intermetallic binary alloys, and by implementing a new data mining technique, we are able to drastically reduce the time necessary to obtain accurate results on novel systems [1]. Furthermore, the huge amount of *ab initio* information contained in the database provides a unique opportunity for comparison with experimental results [2]. The accuracy of state of the art density functional theory pseudopotential methods is addressed in a large scale study of intermetallic systems [2]. [1] S. Curtarolo, D. Morgan, K. Persson, J. Rodgers, and G. Ceder, *Predicting Crystal Structures with Data Mining of Quantum Calculations*, Phys. Rev. Lett. **91**, 135503 (2003). [2] S. Curtarolo, D. Morgan, and G. Ceder, *Accuracy of ab-initio methods in predicting the crystal structures of metals: review of 80 binary alloys*, Calphad (2005)