

MAR07-2006-007215

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Crystal strength by direct computation¹

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The art of making materials stronger goes back to medieval and even ancient times. Swords forged from Damascus steels more than 10 centuries ago possessed a unique combination of hardness and flexibility, two qualities that are difficult to attain simultaneously. The skills of metalworking were based on empirical knowledge and were passed from the master smith to his pupils. The science of physical metallurgy came about only in the XX century bringing with it new methods for finding out why some materials are strong while others are not. Soon it was realized that, when it comes to metal strength, it is all about crystal defects – impurities, dislocations, grain boundaries, etc. - and how they are organized into crystal microstructure. This understanding has since resulted in new effective methods of material processing aiming to modify crystal microstructure in order to affect material's properties, e.g. strength and/or hardness. Remarkably and disappointingly, general understanding that microstructure defines material's response to external loads has not yet resulted in a workable physical theory of metal strength accounting for the realistic complexity of material microstructure. In this presentation I would like to discuss a few tidbits from computational and experimental research in our group at LLNL on crystal defects and their contributions to material strength. My selection of the examples aims to illustrate the major premise of our work that the mechanisms by which the microstructure affects crystal strength are multiple and complex but that there is hope to bring some order to this complexity.

¹This work was performed under the auspices of the US DOE by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.