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Deformation Mechanisms and Manufacturing of Nanostructured Materials Processed by Severe Plastic Deformation (SPD)

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In this project, we focus on 3D nanostructured materials for structural applications where mechanical properties are the primary concern. Several outstanding issues are critical to the development of nanostructured materials and their structural applications. These issues include: i) How do we economically and practically synthesize bulk nanostructured materials? ii) How do we control the vital characteristics, such as nanostructure and the transition from micro- to nanostructure, during synthesis? iii) How do we accurately and appropriately characterize the nanostructures and what are we looking for during the characterization? iv) What are the mechanisms that govern the deformation and, in fact, establish the superior mechanical properties? v) What is the most appropriate theoretical framework for quantitatively describing the nano-, micro-, and macroscopic mechanical response of such materials? These issues are indeed interrelated.

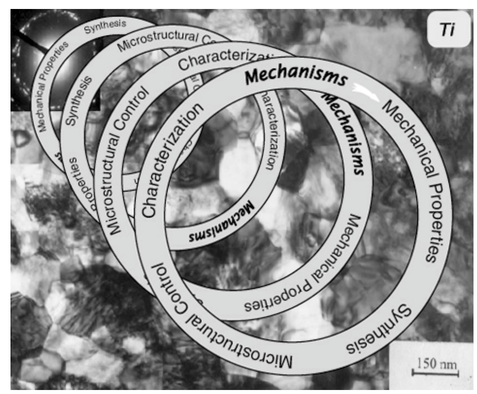
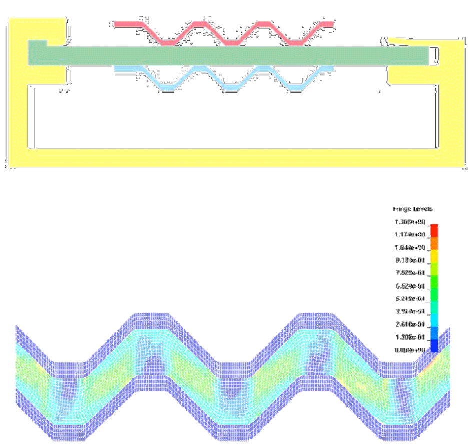
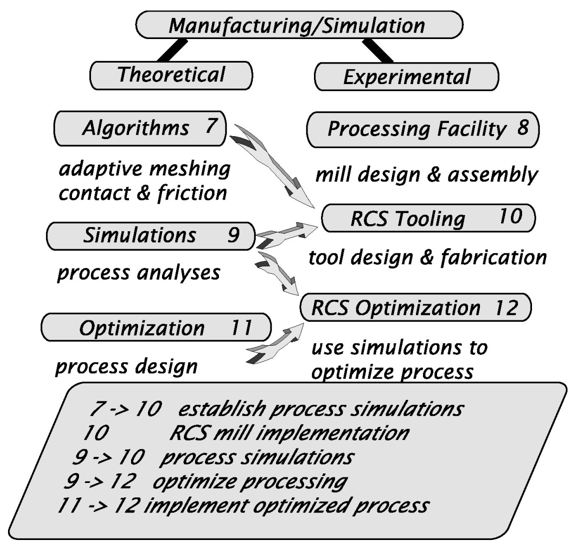


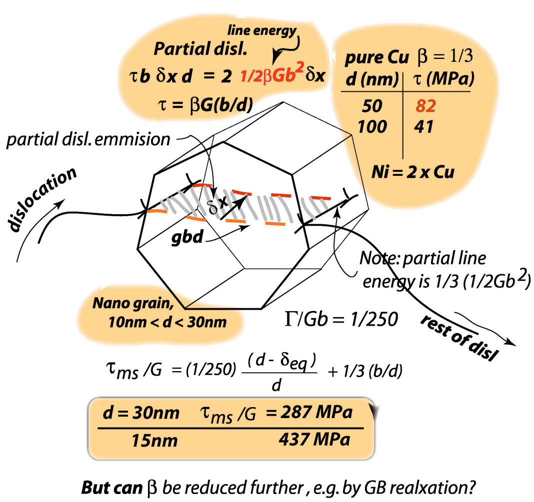
Figure 1 illustrates some of the key areas of focus of our research against a background of a TEM image of nanocrystalline Ti. As shown, we are concerned with developing manufacturing methods, based on processes involving *severe plastic deformation (*SPD), to produce metals and alloys with controlled nano-sized grains, and free from defects such as porosity, cracks, or other atomic scale defects that are known to compromise properties. Our approach involves combined experimental and theoretical (computational) studies aimed at providing a detailed understanding of the relationship between materials chemistry, structure, and properties, and then again to develop the methods for producing optimal structures based on this knowledge.



Manufacturing Science: Figure 2 shows, a finite element simulation, of one of the processes we are developing, namely that of repetitive shear and straightening. Simply put, this process involves subjecting bulk materials to combinations of very intense plastic shear followed by straightening; a key to successful design of such processes involves, *inter alia*, maintaining high degrees of hydrostatic pressure during the shear strain process. This, in turn, involves, design for tooling that imparts optimal combinations of shear and hydrostatic compression. Still another design challenge is to ensure that the deformation is uniform. Our approach involves computational simulation of the entire synthesis process for the purpose of optimization, the results of which are used to design tooling for what is a kind of "rolling process". All aspects of the process are simulated and optimization algorithms are designed to enable a rational approach to optimizing, *inter alia*, the shape of the "gear like" tooling, the temperatures used, deformation rates, and post processing involved with straightening. We have already built a first generation RCS rolling mill and awe are in the process of evaluating its performance *vis-à-vis* these design simulations. The results have been quite encouraging in that uniform grain sizes on the order of 200nm have been synthesized; our immediate goal is to further reduce these to the scale of 50nm[3]. Our ultimate plans involve the construction of a miniature manufacturing facility to demonstrate the viability of the process. In addition, we will conduct detailed studies of the development of structure during the processing and compare these observations to the predictions of our theoretical modeling as well as correlate them with the variables of the processing itself. The various task areas included in our overall manufacturing plan are shown in Figure 3 The interaction between our computational simulations of the RCS process and correlations with our experimental studies of the RCS process are made clear by the linkages. As noted, we intend to build, and fully evaluate, a miniature processing facility based on the combined theoretical/ experimental studies planned herein.

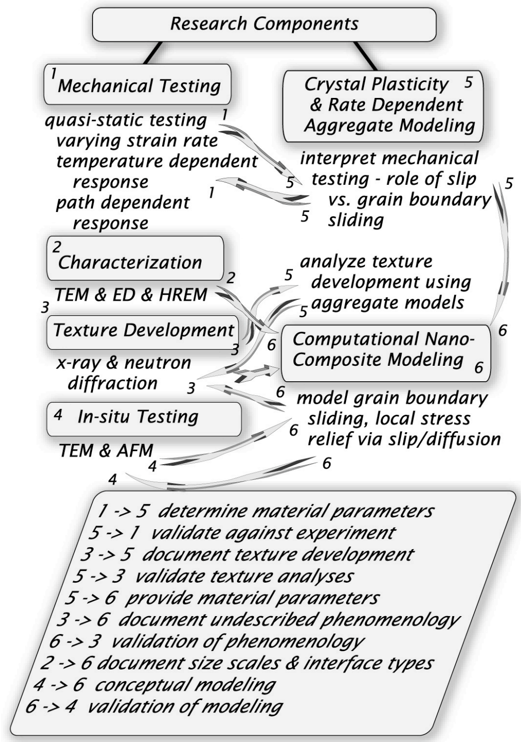


Deformation Mechanisms: When grain sizes fall below the micron size scale the mechanisms of deformation no longer simply involve the processes of slip as is now well established for ductile metals and alloys with traditionally larger grain sizes. We have developed a perspective and framework for describing what turn out to be alternative deformation mechanisms and, indeed, for transitions between alternative mechanisms. Figure 3 illustrates the issue. What we have determined is that when grain sizes fall much below, say 50nm traditional dislocation slip, involving the generation and propagation of intra-grain dislocations. The figure, and the analysis underlying it, illustrates that at such fine grain sizes perfect dislocation emission, from grain boundary triple points, is superceded by the emission of stacking faults (*i.e.* partial dislocations) that traverse the grains as discrete units causing "slip". The process creates stacking faults, and the energetics of this reveals the significance of stacking fault energy as an important parameter in determining the resistance to deformation and thus strength. We have



developed a rigorous constitutive framework for describing this process and are in the process now of implementing our new theories in computational models. We plan to specifically compare our simulated results with detailed measurements made on nanocrystalline Ni. In general the tasks in this area of our research are sketched in Figure 4. As shown, we are conducting both quasi-static as well as dynamic testing on nanocrystalline Ni, Cu, and Ti. Our studies on FCC metals will provide a direct correlation with our recently developed theoretical descriptions of the deformation mechanisms.

At even finer grain sizes still other mechanisms including grain boundary sliding become possible and even preferable to the emission of faults. We have accounted for this in a preliminary fashion, *i.e.* by the formulation of a phenomenological model for grain boundary sliding and have used this model to explore the conditions where dislocation based mechanisms are replaced by grain boundary sliding. Our first model is found in Asaro *et al.* (2003)[1]. A more detailed theoretical development is found in Asaro *et al.* (2003)[2]. The experimental methods employed in this project aside from those already mentioned, include the use of AFM to explore, *in-situ*, grain motion during quasi-static deformation, x-ray diffraction to follow the possible development of deformation textures, and of course TEM ,ED, and HREM to thoroughly characterize the nanocrystalline structures synthesized and studied.



We have, in addition, developed theories for the deformation of ultra-fine grained metals whose grain sizes are on the order of 1 μm and below, *i.e.* that are approaching the nanocrystalline. Such theories are novel in that they specifically account for the effects of dislocation processes such as cross-slip that give rise to convective and diffusive effects in the plastic flow process.

For samples, other links and reprints, see the website hogwarts.ucsd.edu/~nirt., or email rasaro@ucsd.edu.

References:

[1] Asaro, R. J., Krysl, P. and Kad, B., "Deformation Mechanism Transitions in Nano-Scale FCC Metals", to appear in Phil. Mag. Letters

[2] Asaro, R. J., Krysl, P. and Kad, B., Transitions in Deformation Modes in FCC Nanocrystalline Metals, in preparation for publication.

[3] Yuntain Zhu, Asaro, R.J. *et al.*, "Development of Repetitive Corrugation and Straightening", in press, Materials Science and Engineering, January 2003.