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Theoretical Research on Sintering of Metals based on the Results of Molecular Simulations

Introduction

Sintering is the process able to fuse a fine powdered material into a single object, which is of significance because it forms a near net set object reducing wasted material and processing time. Another benefit is that this process occurs below the melting point of the same bulk material, which can save a significant amount of energy needed to manufacture a final product. Here in Houston and Beaumont area, a common use of sintering is laser cladding Stellite™ to valve seats and disks to improve wear resistance. Other uses include the nuclear fuel pellets, crystal lenses, and flexible electronics. While this sintering is of commercial interest, modeling of it is quite complex because of the many contributing factors such as powder size, contamination, molding process and heating method. Efforts have been made modeling different aspects such as density, grain growth, pore distribution and shape. Of interest here, this study uses two models, i.e., the Master Sintering Curve (MSC) and Molecular Dynamics (MD).

The goal is to use data gathered from the MD system as the input information to the MSC model to predict of the bulk material properties primarily grain size, grain growth, elastic strength, and diffusion mechanism:

$$-\frac{dL}{Ldt} = \frac{\gamma\Omega}{kT}\left(\frac{\Gamma_v D_v}{G^3} + \frac{\Gamma_b \delta D_b}{G^4}\right)$$

where *γ* is surface energy, *Ω* is atomic volume, *k* is Boltzmann's constant, *T* is temperature, *Γ* is group of condensed geometric constants, *D* is diffusion coefficient *δ* grain boundary thickness, and *G* is mean grain diameter. The subscripts *v* and *d* delineate whether it is diffusion through the volume or grain boundary, respectively. This equation of the MSC model uses the shrinkage measurements ($-\frac{dL}{Ldt}$) and the thermal history during processing from multiple samples to generate a curve that can be used to predict the behavior of any other samples of the same material (1). For a developed process, the MSC model poses no challenge because the material selection and initially processing is set. However, if a new supplier for raw material must be found or the firing schedule of the component being produced is changed, then developing new materials is particularly expensive in time and resources, especially for the pre-processed or exotic alloy (2,3).

An MD model, however, can perform simulations of most materials under varied conditions, if a suitable molecular potential set exists for the system to be modelled. The primary limitation of a MD simulation is the size because the potential calculates between an atom and each of its neighbors so that the computational load increases dramatically with the simulation size that limits most simulations to the nanometer size of material.

Experiment

The purpose was to combine the best of both models to allow the input information gained from MD simulations of a material to formulate a Master Sintering Curve so that material properties could be predicted in advance of actual processing of samples to save the expense of material at the cost of computer processing time but also allowing the simulation results to be scaled up to bulk material. Material selection started with the ability to find a completed potential system that could be provided to our MD software, LAMMPS (4). Based on our previous work, the potential system has been narrowed to a particular type known as the Embedded Atom Method (EAM) (5) because of its ability to accurately assess the long-range characteristics at the conditions required for sintering. Then, reference data was needed to compare the results to (6). Titanium was chosen due to the large amount of data available as well as its commercial importance. From the reference data, the temperature range was from 800K to 1600K (7), and a set of 10 simulations has been run at 100K intervals in our computational facility.

Results

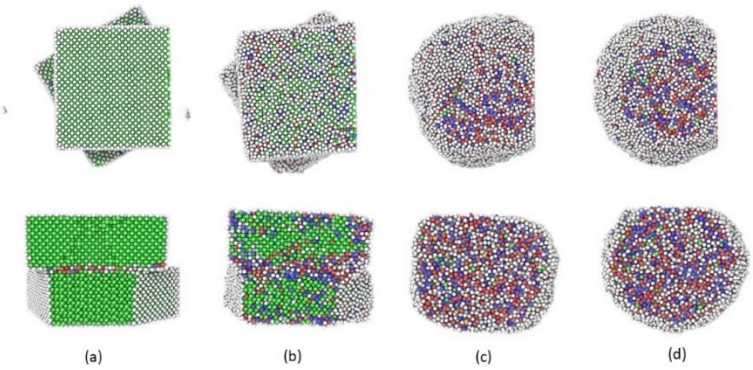

Fig 1: Evolution of material at timesteps: a) 5, b) 100, c)155, d) 235. Given as a top and cut away to see interior colors represent crystal structure: green is fcc, red is hcp, blue is bcp, and white is non-specified

Initially qualitative analysis showed complete fusion of the material and an expected rearrangement and final geometry of the material. With all simulations an MSD calculation was made, and a curve generated and shown in Figure 2. On comparison however, this proved to be a problem that the generated MSD is much higher than the reference values the suspected cause of this is the potential or the MSD calculation and because of the crystal transition very little data exists for the hcp structure of Titanium. The previously stated potential problems can be seen in Figure 1, where the structure rapidly shifts from fcc to both hcp and bcc, and in Figure 3, where the high temperature deviation is obvious as the number of timesteps to complete a begins to rise rapidly. The MSD calculation deviations could be of three possible types: 1) the original bound for the calculation now contains a surface due sphericalization of the grain, which would have an artificially high diffusion due to surface motion, 2) the transition of the crystal structure is being seen as diffusion because the MSD is calculating displacement, and 3) the MSD was made wrong. Because of the EAM and MSD error, the diffusion was never found to be accurate enough to commence MSC curve generation. Due the intense nature of generating an EAM potential, efforts are now underway to validate the MSD made by LAMMPS. LAMMPS makes periodic dump files that contain position and velocity data that will allow for a manual formulation of the MSD and to ensure that a surface wasn't inadvertently captured a new simulation is being developed that only contains bulk material. Later, a new EAM will still need to be reformulated using the right structure and allowance for excited states.

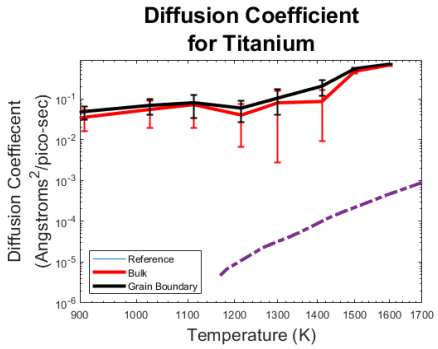

Fig 2: Calculated diffusion Coefficient.

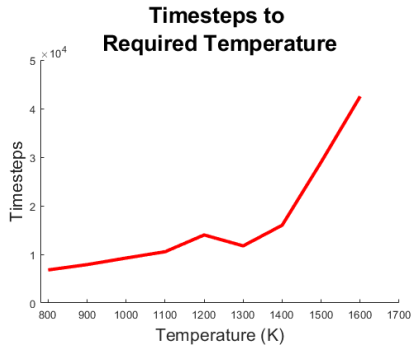

Fig 3: Total timesteps in a simulation.

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