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September 8, 2007

Fifth International Conference on Inertial Fusion Sciences and Applications  
Kobe, Japan  
September 9, 2007 through September 14, 2007

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# Numerical analysis of nanograin collision by classical molecular dynamics

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**Abstract.** We have carried out atomistic simulations of grain-grain collisions for spherical grains of 1.4 and 4 nm radii, with relative velocities of 3.6–6.1 km/s and a number of impact parameters. Since the initial grains are crystallites without any pre-existing defects, grain shattering due to nucleation of cracks was not observed in our simulations. We find grain fusion in some events, but generally melting occurs, leading to nucleation, growth and linkage of voids in the melt, which then leads to production of small clusters. The size distribution does not obey a simple power law and can be considered as having four different regimes, where each regime can be fitted as a power law.

## 1. Introduction

Interstellar dust grains [1] comprise only 1% of the mass in the molecular clouds of galaxies and yet catalyze the formation of many gas phase molecules, in particular H<sub>2</sub> [2], which allows for the cooling and collapse of these clouds and the formation of stars and planets. High-energy radiation and particles from hot stars, supernovae, or active black holes can alter the physical properties of dust grains and thereby affect their role in these processes.

There is no experimental study on grain-grain collisions, for grain smaller than tens of microns, except for clusters with less than 100 atoms. Studies at the mm/cm scale can be roughly understood by continuum models, but these models might break down at the nanometer scale. There are many atomistic molecular dynamics (MD) simulations on the destruction of 3D droplets due to large temperature input [3], 2D solids [4, 5], or collision of disks [6], but there are very few simulations on grain-grain collisions, never going beyond tens of atoms [7, 8].

Here we demonstrate how MD simulations of grain-grain collisions for grain with more than 100 atoms can be used to understand what happens for nanometer-sized grains, colliding at relatively low velocities.

## 2. Numerical Methods

We use classical MD simulations to simulate cluster collisions with the code LAMMPS [9]. Classical molecular dynamics uses Newton's equations of motion to move individual atoms

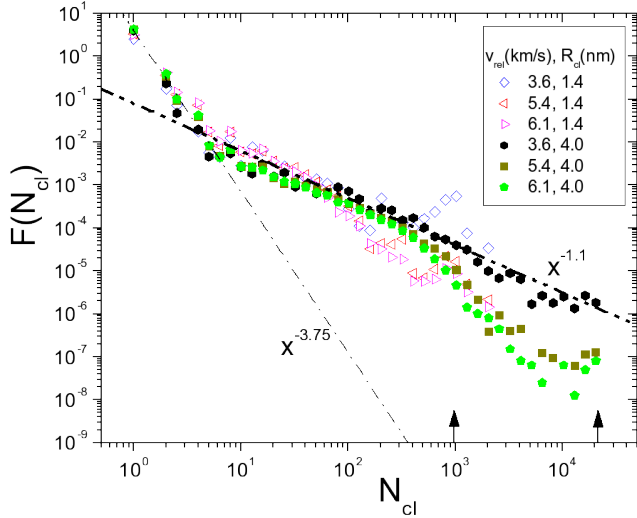
forward in time using an interatomic potential. The potential used here is a many-body potential fitted to reproduce the properties of copper and is intended as a generic example of an interaction potential that could represent metallic glasses as in GEMS. This potential describes defect energetic well, including surface energies, and it was fitted to the equation of state up to high pressures. It has also been shown that it reproduces the shock Hugoniot:  $U_s = c_o + 1.5U_p$ ;  $U_p = v_{\text{rel}}/2$ ;  $P = \rho_o U_s U_p$ . The bulk sound speed is  $c_o = 4$  km/s. Therefore, the relative velocities  $v_{\text{rel}} = 3.6, 5.4,$  and  $6.1$  km/s would correspond to Hugoniot pressures of 1.1, 1.9, and 2.3 Mbars, respectively in an infinite solid for a steady shock wave. These values give an upper limit to the transient pressure in our finite system.

The potential used here also reproduces the experimental shock melting of copper [10], which occurs at a relative velocity of  $\sim 6$  km/s for an infinite system ( $P \sim 2.2$  Mbars). A pressure of 30 GPa is needed to produce homogeneous nucleation of dislocations ( $v_{\text{rel}} = 1.5$  km/s). Spall from a free surface occurs only for pressures close to shock melting [11], but void nucleation can occur inside the material at pressures of  $\sim 50$  GPa due to collision of rarefaction waves from two free surfaces. We note that at velocities well above shock melting electronic effects might play a role, and they are not included in our classical simulations.

We approximate the clusters as spherical particles of several radii,  $R_{\text{cl}}$ , but here we focus on two:  $R_{\text{cl}} = 1.4$  and  $4$  nm. This leads to clusters with  $N_{\text{atoms}} \sim 1060$  and  $22500$  atoms each respectively. The two clusters are positioned at some distance larger than the interaction radius of the interatomic potential (0.55 nm), equilibrated at 10 K, and then given a relative velocity of 3.6, 5.4, or 6.1 km/s. We have carried out simulations for five impact parameters  $b$ ,  $b/R_{\text{cl}} = 0.0, 0.2, 0.4, 0.6,$  and  $0.8$ . Our clusters are crystalline (and therefore anisotropic). In order to avoid artificial alignment of the crystals during the collision, we rotate the clusters at some random orientations and repeat the simulations for 5–10 different orientations at each impact parameter. Therefore, we have 50 simulations at each velocity for the small clusters and 25 for the large clusters. We note that the results are not heavily dependent on orientation, and that amorphous grains would behave similarly, especially in collisions where melting dominates cluster production as in most of the cases simulated here. Simulations are followed during tens of ps, until the size distribution of the resulting clusters does not change ( $\sim 40$ – $70$  ps), except for a handful of monomers being emitted from some large hot clusters. Radiative cooling is not included in MD simulations and it will not occur until microseconds after the collision occurred.

### 3. Results

Figure 1 shows the size distribution of the final cluster distribution for all cases. The case of  $R_{\text{cl}} = 1.4$  nm can lead to fusion of the grains, given by the clusters of size  $N_{\text{cl}}/N_{\text{atoms}} = 2$ . This is the most probable outcome for  $v_{\text{rel}} = 3.6$  km/s for  $b = 0.0$ . Another likely outcome is the scattering of the grains for large impact parameter (grazing collisions). This leads to the peak at  $N_{\text{cl}}/N_{\text{atoms}} = 1$ , which also occurs for  $R_{\text{cl}} = 4$  nm. Note also the presence of cases when only 3–4 major fragments are produced. It is generally assumed that the resulting size distribution follows a power law dependence. This is indeed the case in shattering simulations and experiments at the mm/cm scale [6] and also for thermal destruction of droplets [3], fracture of 2D solids [4, 5]. Deviations to the power scale behavior are often seen for the smallest/largest clusters. Here we observe something extremely different. The distribution follows a power law with exponent  $\sim -1.1$  for cluster sizes of 5–8 atoms up to  $0.04N_{\text{atoms}}$ . For smaller clusters it follows a power law with an exponent of  $\sim 3.75$ . For clusters in the range  $\sim 0.04$ – $0.1N_{\text{atoms}}$  it seems to roughly follow also a power law with exponents that vary in the range  $\sim -1$  to  $-4$  depending on cluster size and energy, to grow at larger cluster sizes and produce peaks due to scattering and fusion. Note that even at the highest relative velocity, the number of clusters is low compared to the total number of atoms, i.e., the multiplicity of the event [12] is low ( $\sim 0.3$  for small clusters at 6.1 km/s).



**Figure 1.** Final cluster size distribution. Arrows indicate original cluster size. Note that the bins are logarithmic in size.

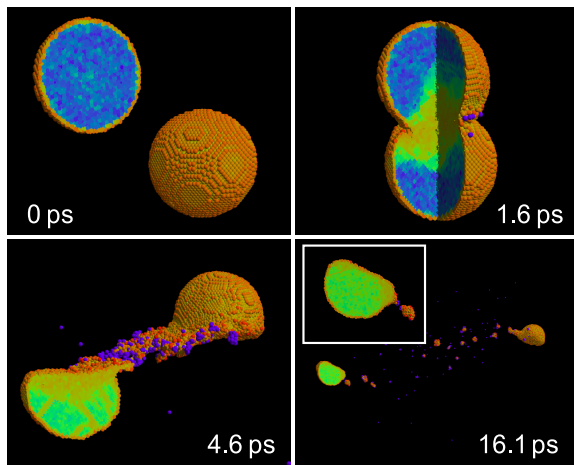
Figure 2 shows snapshots of a collision for  $R_{cl} = 4$  nm,  $b/R_{cl} = 0.8$ , and  $v_{rel} = 5.4$  km/s. Note that the clusters graze each other tearing apart a thin liquid film along the contact surface. Voids are nucleated in the film, which then breaks into small clusters, leaving the original grains nearly intact. The shock wave propagates inside the grain. Because of the grain crystallinity the shock front is not hemispherical. The wave nucleates dislocations, seen as line defects, but the recovery of the sample leads to annealing of the dislocations, leaving grains which are still single crystals without any “bulk” defects, with the possible exception of twin boundaries, which are relatively easy to produce for this potential.

Figure 3 shows snapshots of a head-on collision for  $R_{cl} = 4$  nm,  $b/R_{cl} = 0.0$ , and  $v_{rel} = 5.4$  km/s. Note that the two clusters flatten upon collision, leading to a hot outer ring where small clusters are “evaporating”. The liquid “pancake” is expanding, and, therefore, voids nucleate, grow, and link until multiple clusters are produced. The resulting clusters are a mixture from both original clusters, unlike the case for  $b/R_{cl} = 0.8$ , where most of the mass of the clusters remains in the original clusters unmixed except in the few small cluster produced.

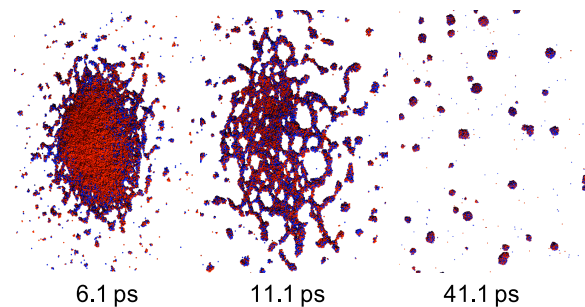
#### 4. Discussion and Summary

Our simulations show that collisions of nanometer scale grain can differ significantly from collisions at a larger scale. Our grains are defect free. This is a realistic scenario, given that dislocations and other defects would likely disappear at the surface. It has been shown that metallic nanomaterials are typically defect-free below  $\sim 10$ – $50$  nm. Grain boundaries would be unlikely at this small scale, except for twin boundaries. Our simulations imply that even strong collisions would lead to final fragments which would be defect free. We note that melting of the grains might lead to a final cool cluster that will be crystalline or amorphous depending on the details of the interatomic potential. Metallic, single component systems like the one simulated here will likely re-crystallize into a single crystal, while other materials like SiC would likely lead to a large amorphous component.

Because these materials are defect free, grains do not shatter into smaller clusters, as shown in studies at larger scales [6, 13]. Instead, low velocities lead to fusion or scattering, with only a small production of clusters, much less than 1% of the grain size in mass. Larger velocities lead to melting and cluster production by void nucleation. This resembles the cluster production of materials by laser ablation [14, 15, 16], and the result is a cluster size distribution with a power law behavior and exponent  $\sim 1$  over 1–3 orders of magnitude in cluster size, unlike typical



**Figure 2.** Time evolution of a grazing collision with  $R_{cl} = 4$  nm,  $b/R_{cl} = 0.8$ , and  $v_{rel} = 5.4$  km/s. Coloring using the centrosymmetry parameter [17].



**Figure 3.** Time evolution of a head-on collision with  $R_{cl} = 4$  nm,  $b/R_{cl} = 0.0$ , and  $v_{rel} = 5.4$  km/s. The scale of the frames increases with time in order to show all clusters.

power law distributions due to fracture and crack percolation. We also note that, if nm grains are retrieved in future space missions, the fact that they are defect free or crystalline would not necessarily indicate that they did not experience strong grain-grain collisions during their evolution.

Preliminary simulations using amorphous carbon grains (with the Brenner potential), also show fusion and scattering for velocities up to 7 km/s, demonstrating that the nanometer scale can display significantly different behavior than the continuum scale. Therefore, grain-shattering models reaching down to clusters with tens of thousands of atoms or less have to be revisited.

The work at LLNL was performed under the auspices of the U.S. Department of Energy (DoE) and Lawrence Livermore National (LLNL) Laboratory under contract No. W-7405-Eng-48. This research was performed at Thunder, a LLNL supercomputer.

## References

- [1] Draine B T 2003 *Annu. Rev. Astro. Astrophys.* **41** 241
- [2] Hollenbach D and Salpeter E E 1971 *Astrophys. J.* **163** 155
- [3] Strachan A and Dorso C O 1997 *Phys. Rev. C* **56** 995
- [4] Holian B L, Germann T C, Maillet J-B and White C T 2002 *Phys. Rev. Lett.* **89** 285501
- [5] Diehl A, Carmona H A, Araripe L E, Andrade Jr. J S and Farias G A *Phys. Rev. E* **62** 4742
- [6] Kun F and Herrmann H J 1996 *Int. J. Mod. Phys. C* **7** 837
- [7] Lejeune A, Perdang J and Richert J 2003 *Phys. Rev. E* **67** 046214
- [8] Yamaguchi Y and Gspann J 2002 *Phys. Rev. B* **66** 155408
- [9] Plimpton S 1995 *J. Comp. Phys.* **117** 1; <http://lammmps.sandia.gov/>
- [10] Bringa E M, Cazamias J U, Erhart P, Stölken J, Tanushev N, Wirth B D, Rudd R E and Caturla M J 2004 *J. Appl. Phys.* **96** 3793
- [11] Germann T C 2006 *Int. J. Impact Eng.* **33** 285
- [12] Campi X 1988 *Phys. Lett. B* **208** 351
- [13] Kun F and Herrmann H J 1999 *Phys. Rev. E* **59** 2623
- [14] Gilmer G H *et al* 2004 unpublished
- [15] Zhigilei L V 2003 *Appl. Phys. A* **76** 339
- [16] Urbassek H M 1988 *Nucl. Instrum. Methods Phys. Res. B* **31** 541
- [17] Kelchner C L, Plimpton S J and Hamilton J C 1998 *Phys. Rev. B* **58** 11085