

Letter

Compaction and plasticity in nanofoams induced by shock waves: A molecular dynamics study



Nina Gunkelmann^a, Yudi Rosandi^b, Carlos J. Ruestes^c, Eduardo M. Bringa^c, Herbert M. Urbassek^{a,*}

^a Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

^b Department of Physics, Universitas Padjadjaran, Jatinangor, Sumedang 45363, Indonesia

^c CONICET and Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Cuyo, Mendoza 5500, Argentina

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ABSTRACT

Shock waves are produced in Al nanofoams by a piston moving with velocity U_p . They induce plastic activity in the ligaments before eventually the foam structure is crushed and a compact material results. We demonstrate dislocation formation in the foams and correlate it with the velocity and stress profiles in the shock wave. The profiles exhibit a 3-wave structure indicating 3 wave regimes: elastic precursor, plastic activity in the ligaments, and foam crushing. The shock wave velocity V follows well macroscopic predictions, $V \propto U_p$. The length of the non-collapsed part of the foam is well described by an analytical compaction model.

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1. Introduction

Metal foams receive high interest due to their light weight and high stiffness [1]. Applications range from automotive industry [2] to space science where foams may become important as radiation shields [3]. The possibility of achieving light-weight yet high-strength nanofoams make them promising candidates for their application to high-velocity impact loading conditions [4,5].

However, the mechanisms of shock response of foams – in particular nanofoams – are still not fully understood. Most experimental and simulation studies deal with macroscopic metal or plastic foams [6–8]. Finite-element models are widely used to explore stress–strain curves for metal foams [9,10]. Theoretical analysis has provided a macroscopic model of the propagation of stress waves in cellular solids [10] as well as of one-dimensional plastic shock waves [11,12]. Lopatnikov et al. investigated analytical solutions for dynamic deformation and energy absorption of foam materials under plate impact conditions under simplified materials models [13–15]. These models have been further refined in recent years to understand the dynamics of foam compaction under compression [9–17].

Molecular dynamics (MD) simulation offers a tool to investigate the atomistic response of foams to the passage of a shock wave. Zhao et al. [18] considered shock induced melting and found internal

jetting producing shock front roughening [18]. Rodriguez-Nieva et al. [19] studied the plastic deformation of nanoporous fcc metals using MD and dislocation analysis and found that nanovoid surfaces act as effective sources for dislocations. Sun et al. [20] investigated the plastic response of a nanoporous Au foam to uniaxial tensile deformation on an atomistic level and Ngo et al. [21] reported on the immediate onset of plastic yielding at the smallest loads. Finally, Farkas et al. [22] used MD to study the compaction mechanisms under compression and tension. Jian et al. [23] and Zhao et al. [24] studied shocks in nanoporous Cu foams with pore size and ligament thickness of around 3.5 nm; these studies focused on the melting behavior induced by pore collapse. Also the work of Souillard et al. [25] studied shock-induced melting in Cu foams and related it to the plastic work done during pore collapse.

In the present paper we use MD simulations to study the propagation of shock waves through an Al nanofoam. We characterize the structure of the shock wave in its velocity, stress and density changes. In front of the crushing regime in which the foam material is compressed to almost bulk density, we characterize a plastic regime, in which dislocations are created in the foam ligaments. The length of the non-collapsed part of the foam as well as the shock-wave velocity can be described by simple models.

2. Simulation method

In the present paper we use MD simulations to study the propagation of shock waves through an Al nanofoam. We

* Corresponding author.

E-mail address: urbassek@rhrk.uni-kl.de (H.M. Urbassek).

URL: <http://www.physik.uni-kl.de/urbassek/> (H.M. Urbassek).

construct foams with different initial filling factors varying from $\phi_0 = 0.15$ to $\phi_0 = 0.75$. The construction algorithm makes use of the non-simply connected structure of atoms of defined temperature in a liquid. In detail, we first create a template for the foam structure by starting with an fcc crystal with periodic boundary conditions. The atoms interact with a simple Lennard–Jones (LJ) potential. The target crystal is heated above the melting point for several thousand time steps to establish thermal equilibrium. Due to equilibrium fluctuations not all atoms have the same temperature. From the melt all atoms with temperature above a chosen value are removed, until the desired filling factor is met. In this stage we obtain a spongy structure, which mimics a nanofoam; however, some atoms are isolated inside voids. In order to attach them to ligaments, we relax the structure using a short-ranged LJ potential with a strongly increased binding energy. Finally, all non-connected atoms and clusters are stripped off by using a cluster detector [26] which isolates the largest interconnected structure. This structure is used as template to create the actual crystalline Al foam by using it as a spatial filter to remove all superfluous atoms from an fcc Al crystal. At two opposing surfaces we fix full-density ends of 15 nm length to the foam, which can be used as piston. We note that the use of such ‘sandwiched’ foam structures is widespread [27]. The average ligament size is around 2.5 nm. An example of the structures formed is given in Fig. 1(a). The foams have a rod-like shape with a long axis – denoted by z in the following – of 156 nm in total and lateral dimensions of 13 nm. The Al crystal has a $\langle 100 \rangle$ orientation with respect to the shock direction. We apply periodic boundary conditions in lateral direction and free boundaries along the shock direction. We relax the samples using high-temperature annealing at 80% of the melting temperature for 100 ps [28]. We note that for the thinnest foam ($\phi_0 = 0.15$) we had to skip this last step since it made the foam collapse. The shock wave simulations are conducted at a temperature of 10 K in order to minimize thermal noise. The open-source MD code LAMMPS [29] is used in this work to perform the simulations. For our simulations we employ the interatomic potential for Al developed by Mendelev et al. [30].

We obtained local von-Mises stresses inside the foam before and during the shock from the local atomic virials as determined within the LAMMPS software. Evidently, stresses increase during loading, but the maximum local stress was around 15 GPa; this is far above the macroscopic stresses measured as averages in the specimen in Fig. 3 below, since local stresses concentrate in the ligaments. This analysis justifies our use of the potential by Mendelev et al. [30], since the dependence of the elastic constants under pressure is realistic in this pressure regime. We note, however, that recently Al potentials have been set up that are designed to perform realistically in particular under shock conditions [31].

Shock waves are generated by the so-called piston-driven algorithm [33,34] by giving a certain particle velocity U_p in z direction to the atoms in a thin slab (thickness of one lattice constant) on one side of the sample. Note that these atoms are not subjected to the forces of the surrounding atoms. The remainder of the system volume is simulated under NVE conditions. We consider piston velocities varying from $U_p = 0.1$ to $U_p = 0.9$ km/s. The piston velocity is increased linearly from 0 to its maximum value U_p during a ramp loading time of 15 ps and then held constant. The simulation is continued up to a total time of 80 ps.

To evaluate the results we determine various material properties in dependence of the z position in the foam. These profiles are determined by dividing the sample into small slabs with a thickness of 1.215 nm along the z direction. We calculate the velocity profile in z direction, v_z , the stress in z direction, p_{zz} , the relative density, ϕ , the temperature, T , and the shear stress, p_{shear} . The latter is defined as

$$p_{\text{shear}} = \frac{1}{2}(p_{zz} - p_{\text{trans}}), \quad (1)$$

where p_{ij} denote the components of the stress tensor, and the transverse stress is defined as

$$p_{\text{trans}} = \frac{1}{2}(p_{xx} + p_{yy}). \quad (2)$$

We measure the filling factor ϕ by counting the number of atoms in each slab normalized to the bulk density in Al.

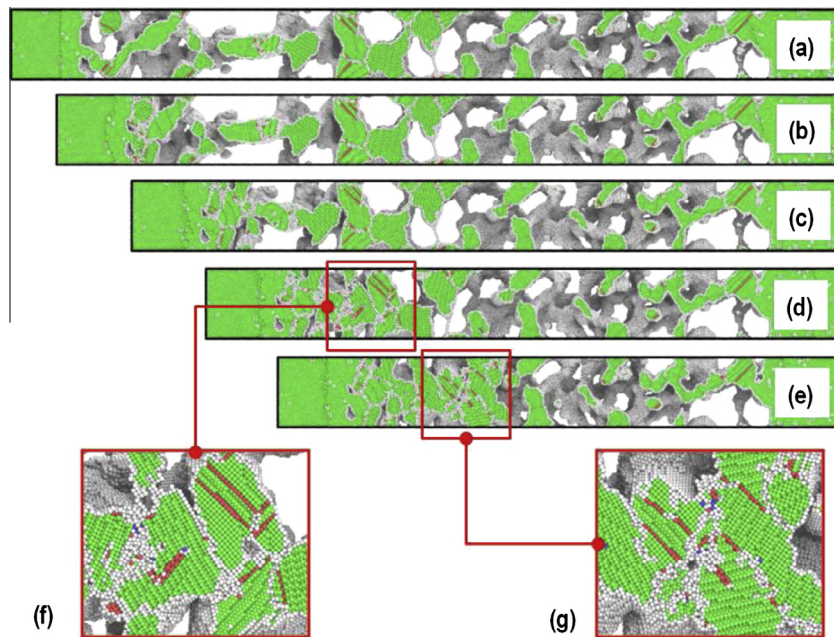


Fig. 1. Snapshots of the sample with filling factor $\phi_0 = 0.25$ at times of (a) 0 (b) 20 (c) 40 (d) 60 (e) 80 ps. (f) and (g) provide detailed views as indicated in the plot. The simulation is performed for a piston speed of $U_p = 0.7$ km/s. The shock wave runs from left to right. Local atomic structures are identified by adaptive CNA [32]. Green: fcc; red: hcp; blue: bcc; gray: without defined structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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