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MD SIMULATIONS OF LASER-INDUCED ULTRASHORT SHOCK WAVES IN NICKEL

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Abstract. The dynamics of ultrashort shock waves induced by femtosecond laser pulses were explored in nickel-glass and free-standing nickel films by molecular dynamics simulations. Ultrafast laser heating causes stress-confinement, which is characterized by formation of a strongly pressurized 100-nm-thick zone just below the surface of the film. For low-intensity laser pulses, only a single elastic shock wave was formed despite pressures several times greater than the experimental Hugoniot elastic limit. Because the material remains uniaxially compressed for < 50 ps, comparatively slow processes of dislocation formation are not activated. For high intensity laser pulses, the process of double wave breaking was observed with formation of split elastic and plastic shock waves. Presence of a trailing rarefaction wave acts to attenuate the plastic wave until it disappears. Agreement between the experimental and simulated Hugoniot was facilitated by a new EAM potential designed to simulate nickel in a wide range of pressures and temperatures.

Keywords: femtosecond laser, shock wave, molecular dynamics
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INTRODUCTION

Over the last several years, irradiation by ultrashort laser pulses has emerged as an efficient generator of shock waves with durations on the order of several tens to hundreds of picoseconds [1–4]. In particular, shock waves generated by femtosecond laser pulses, which have durations on the order of many atomic-scale processes, provide a unique opportunity to probe the response of materials to extreme conditions. A joint experimental [2] and computational [5] work investigated such ultrashort shock waves in thin aluminum films using femtosecond laser pulses with duration 150 ps. Results of these investigations indicated that the observed shock waves were most likely elastic despite amplitudes exceeding the commonly accepted value for the Hugoniot elastic limit (HEL) in metals ∼ 1 GPa.

In another experimental work [1], shock waves were generated in thin nickel films deposited on glass by low-energy 0.2 – 0.5 mJ femtosecond laser pulses with similar duration 130 fs. Making use of frequency-domain interferometry, precise measurements of the rear side response of the film upon arrival of the shock wave were obtained with subpicosecond resolution. As in the previous case, there were several indications, which will be discussed in detail later, that the observed shock waves were elastic. By performing complementary molecular dynamics simulations of nickel films on glass, the first of this two part work will address the structure of the shock waves observed in Ref. [1].

Because the driving laser pulse is transmitted through glass before being incident on the nickel film, there is a limit on the intensity of the pulses that can be used. Above this limit, optical breakdown of the glass occurs and the resultant plasma prevents any energy transmission to the metal surface. There-
Results from shock wave simulations are plotted in wide ranges of pressures and temperatures [6]. We developed a new embedded atom method (EAM) interatomic potential for nickel specifically designed for nickel in the [110] direction. Our simulations employed a femtosecond laser pulse to transfer its energy to the conduction electrons within the skin layer (∼10 nm). Within a time $\tau_e \sim 10$ ps, the high-temperature electrons penetrate to a depth of $d_T$ and thermalize with the surrounding cold ion subsystem. Since $\tau_e < \tau_i$, where the acoustic time $\tau_i = d_T/c_s$, the heating is approximately isochoric, which leads to stress-confinement in a 100-nm-thick layer near the surface of the nickel film. The early stages, including laser energy deposition and electron-ion energy exchange, were simulated by a two-temperature hydrodynamics (2T-HD) code, which yielded the temperature distribution of the crystal after electron-ion thermalization. The 2T-HD temperature distribution was then fit to a one-dimensional Gaussian function $T(x)$. Using $T(x)$ as the target function for a Langevin thermostat that runs until $\tau_{ie}$, the femtosecond laser heating was effectively reproduced in MD simulations. Different fluences were simulated by adjusting the maximum temperature at the film’s surface $T(0)$. In addition, HD simulations were performed in which the nickel

SIMULATION TECHNIQUE

Our simulations are directly related to the experiment reported in [1], where thin nickel films were deposited onto a ∼150 μm glass substrate. Single-crystalline nickel samples oriented in the [110] direction with a vacancy concentration of 0.1% deposited on a thin (∼250 nm) layer of glass were simulated. To minimize the complexity of the calculations, the glass was approximated by the same nickel crystal with reduced density $\rho = 0.047\rho_{Ni}$ chosen so as to reproduce the acoustic impedance $Z = c_s\sqrt{\rho/\rho_{Ni}}$ of glass, where $c_s$ is the longitudinal sound speed of nickel in the [110] direction. Our simulations employed a new embedded atom method (EAM) interatomic potential for nickel specifically designed for use in wide ranges of pressures and temperatures [6]. Results from shock wave simulations are plotted in Fig. 1 against experimental data [7]. Good agreement along the plastic branch ensures that the new EAM potential accurately describes the response of nickel to shock compression.

In the first stage of heating, the femtosecond laser pulse transfers its energy to the conduction electrons within the skin layer (∼10 nm). Within a time $\tau_e \sim 10$ ps, the high-temperature electrons penetrate to a depth of $d_T$ and thermalize with the surrounding cold ion subsystem. Since $\tau_e < \tau_i$, where the acoustic time $\tau_i = d_T/c_s$, the heating is approximately isochoric, which leads to stress-confinement in a 100-nm-thick layer near the surface of the nickel film. The early stages, including laser energy deposition and electron-ion energy exchange, were simulated by a two-temperature hydrodynamics (2T-HD) code, which yielded the temperature distribution of the crystal after electron-ion thermalization. The 2T-HD temperature distribution was then fit to a one-dimensional Gaussian function $T(x)$. Using $T(x)$ as the target function for a Langevin thermostat that runs until $\tau_{ie}$, the femtosecond laser heating was effectively reproduced in MD simulations. Different fluences were simulated by adjusting the maximum temperature at the film’s surface $T(0)$. In addition, HD simulations were performed in which the nickel

FIGURE 1. (Color online) $P-V$ Hugoniot for single-crystalline Ni with SW propagation in the [110] direction. Squares are simulated points along the elastic branch and circles along the plastic branch. Crosses were taken from an experimental database [7]. Position of HEL corresponds to samples with a vacancy concentration of 0.1%. Dashed line gives the metastable extension of the elastic branch to HEL. The transition and electron-ion energy exchange, were simulated by a two-temperature hydrodynamics (2T-HD) code, which yielded the temperature distribution of the crystal after electron-ion thermalization. The 2T-HD temperature distribution was then fit to a one-dimensional Gaussian function $T(x)$. Using $T(x)$ as the target function for a Langevin thermostat that runs until $\tau_{ie}$, the femtosecond laser heating was effectively reproduced in MD simulations. Different fluences were simulated by adjusting the maximum temperature at the film’s surface $T(0)$. In addition, HD simulations were performed in which the nickel

FIGURE 2. (Color online) Snapshots from molecular dynamics (MD) simulation of elastic wave propagating in [110] direction through 839 nm nickel film. The process of wave breaking takes a considerable amount of time and the shock front is not fully formed until reaching the edge of the sample.
results and discussion

As the stress-confined state decomposes, a strong compressive wave is formed, which propagates through the target. In our MD simulations, the compressive wave eventually broke into a weak elastic shock wave, as shown in Fig. 2. As is evident from the figure, the process of wave-breaking was relatively slow and a fully-formed shock front was only realized for the thickest (839 nm) film. The relative arrival times and rear side displacements of the shock waves from experiment and MD simulations are shown in Fig. 3. Both experiment and MD give similar profiles and arrival times, whereas the strong plastic shock wave simulated by HD arrives significantly later and produces a much larger displacement. Simulated rear side velocities for an 839 nm film are shown in Fig. 4. Using the acoustic approximation, the simple transformation $u(x) \rightarrow V(t)$ applied to the MD simulation data, yields a velocity profile which agrees well with that directly obtained from the rear surface.

Two methods were used to measure the shock velocity $u_s$ in experiment: in the first, an average value for $u_s$ was directly measured from shock wave propagation times and, in the second, the maximum particle velocity $u_p$ in the shock wave at the rear surface was measured and $u_s$ was calculated from the plastic branch of the Hugoniot $u_s = 4.60 + 1.437u_p$. For a free surface, $u_p$ is half of the maximum surface velocity $u_b = 2u_p$. The first method gives a value for $u_s$ of $6.15 \pm 0.39$ km/s in 839 nm film, which is comparable to the MD result of $6.22$ km/s; whereas the second method yields a significantly smaller shock velocity of $4.80 \pm 0.02$ km/s. Simulated and experimental values for $u_p$ for two film thicknesses are given in Fig. 3. Experimental values for the maximum rear surface velocity, and by extension $u_p$, were obtained by linear fits to the rear side displacement data after shock wave arrival, shown in Fig. 3.

Agreement with MD results and the absence of shock wave splitting suggest that the waves observed in [1] are, in fact, purely elastic. In turn, this explains why the value for $u_s$ obtained by the second method was significantly lower than that obtained by the first. It should be noted that attenuation of the relatively weak shock as it propagates through the sample has a small effect on the velocity measured at the rear.
that split elastic and plastic shock waves form for pressures > 50 GPa. The process of double wavebreaking is illustrated in Fig. 5. Due to the rarefaction tail, the plastic wave attenuated as it propagated through the sample. Once the amplitude of the plastic wave dropped below 50 GPa, then plastic deformation stopped and only an elastic wave remained. In principle, it is therefore possible to localize plastic deformation to a specific depth by simply adjusting the intensity of the incident laser pulse. This is similar to the observation in previous MD simulations of a localized polymorphic phase transition induced in a model diatomic molecular solid by hypervelocity impacts of ultra-thin flyer plates [9].

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