CHAPTER 4

What is a Shock Wave?
—The View from the Atomic Scale

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It is easy to say that everything starts at the time and distance scale of atoms. Strong shock waves provide the most appropriate conditions under which to study processes at the atomistic level on the computer. In the last three decades, molecular-dynamics (MD) simulations have been applied to shock waves in gases, liquids, and solids. In the case of solids, the problem becomes more complicated because of defect structures, which have an intrinsically larger length scale than that of the mean atomic spacing. In sufficiently strong shocks, defects can be produced homogeneously. For weak shocks, they can be triggered as the wave interacts with pre-existing defects that serve as inhomogeneous nucleation sites.

In all cases, the critical feature of nonequilibrium MD (NEMD) simulations is the time it takes to attain a steady wave, beginning at the time of impact. As larger and larger samples have become feasible with large-scale, massively parallel NEMD, the level of complexity has increased dramatically, to include the possibility of structural phase transformation, as well as plastic deformation, and chemical reaction for molecular systems.

The biggest challenge for the future is the approach to modeling truly meso-scale features, such as exhibited in weak shocks in polycrystalline samples with grain sizes above the micrometer scale, and the simulation of detonations for complex molecules with large reaction zones. However, similar to expected refinements in experimental techniques, advances in atomistic simulations will allow us to probe even further the limits to our fundamental understanding of shockwave phenomena.

4.1. Introduction

The time and distance scales of shock-wave processes, caused by high-velocity impacts, are ideal for investigation at the atomistic level. Molecular-dynamics (MD) simulations, where Newton’s equations of motion for large numbers of strongly interacting atoms are solved on the computer, have been employed to
study shock waves for over thirty years [1], but most successfully in the last
decade, when massively parallel computers have become available.

Strong shock waves in dense fluids can exhibit the steepest rises in density,
velocity, pressure, and energy, with widths as little as a couple of mean atomic
spacings (nearest-neighbor distances in solids and dense liquids are typically of
the order of 0.3 nm). Because shock velocities are supersonic in the uncom­
pressed medium, and because sound speeds are of the order of 6,000 m/s, the
risetime of the shock can be as short as a vibrational period in the solid (or mean
collision time in the fluid), which is of the order of 0.3 ps. These are extremely
tiny time and distance scales, which are dictated by the puny sizes of atoms.
These facts of life were known a century ago, that is, that matter is made up of
atoms, and that atoms are incredibly tiny.

Avogadro’s number of atoms (about $10^{24}$) in a typical metal is contained in a
cube whose side length is about 3 cm, the scale of a typical laboratory shock­
wave experimental sample at a firing site. It is no wonder that engineers doing
continuum-mechanical simulations of such experiments have long felt that ato­
mistic simulations could never possibly have any relevance to the “real world.”
The gap between the continuum, where matter is treated as though it is infinitely
divisible and smooth, and the atomistic, which is as grainy and discontinuous as
matter can get (beyond subatomic particles), is worth quantifying, so that we can
see just how far apart these world views really are.

At the atomistic level, it has been historically evident, time and time again,
that the continuum presses in upon atoms at surprisingly small time and distance
scales. When, in the late 1950s, Berni Alder [2] first carried out equilibrium MD
simulations for hard disks in two dimensions (2D) and hard spheres in 3D, many
scoffed at his notion that a few tens of atoms, or at most a hundred, could exhibit
anything resembling the thermodynamic limit, thought to be something far
closer to $10^{24}$ atoms or molecules. Later, at the end of the 1960s, Alder demon­
strated that hydrodynamic behavior of dense fluids [3] could be ascribed to a
hundred hard spheres, on a time scale of a few mean collision times, and on a
distance scale of a couple of neighbor shells, or mean atomic spacings. In fact,
the fundamental assumption that Boltzmann was forced to make, because he did
not have computers available in 1900, was “molecular chaos,” the exponential
loss of a particle’s memory of its collisional history. Molecular chaos made it
possible to solve the problem of gas dynamics for the velocity distribution func­
tion, which came to be known as the Boltzmann Equation [4]. Molecular chaos
was shown by Alder to be wrong precisely because atoms “remember” their
previous velocity history much better than Boltzmann assumed, by a power-law
decay, rather than exponential. The path to that discovery was the demonstration
of hydrodynamic behavior at the atomic scale.

Near the beginning of the 1970s, Bill Hoover (who had come to the
Livermore Lab to work as a postdoc of Berni’s) pioneered the method of non-