

Search for Viable Thermoelectric Materials

Anthony Frachioni, Bruce White, Binghamton University

State University of New York Energy: A universal issue

According to the US Energy Information Administration, world marketed energy consumption is projected to increase by 49 percent from 2007 to 2035 (this assumes no new laws or policies are put in place). This increase in demand will put incredible stress on today's energy sources, most of which still rely on non-renewables like coal and oil. In addition to the harm this will do to our natural environment, the global economy will suffer from a severe general lack of energy supply. This problem motivates a search for renewable, efficient, inexpensive energy sources.

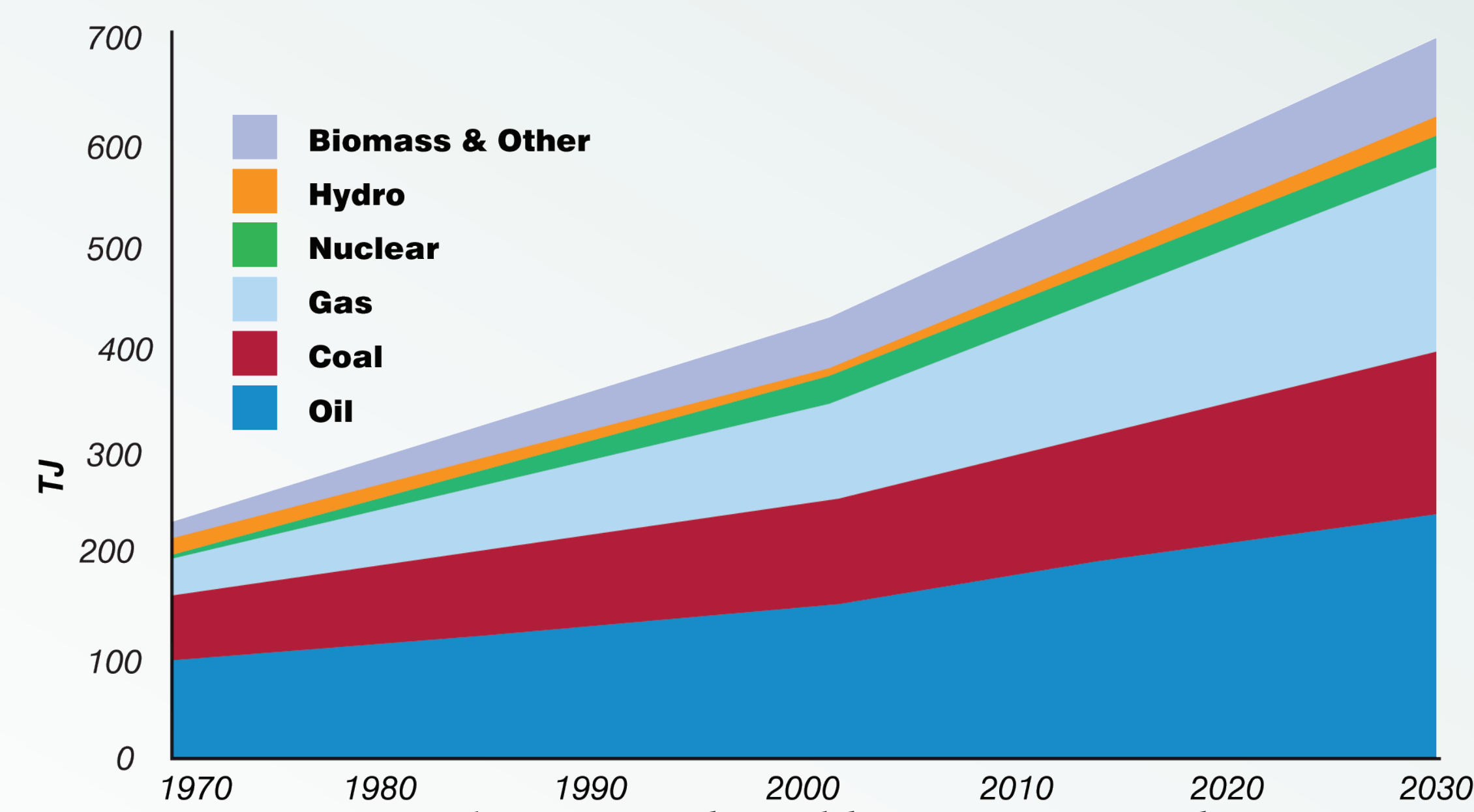


Figure 1: Projected World Energy Demand
OECD/IEA World Energy Outlook 2010

Heat energy is abundantly available in many contexts globally. Anytime energy is harvested, transported, or used, nature insists that some be lost to heat. Our sun supplies a constant source of energy; some also have taken advantage of heat energy which collects underground.

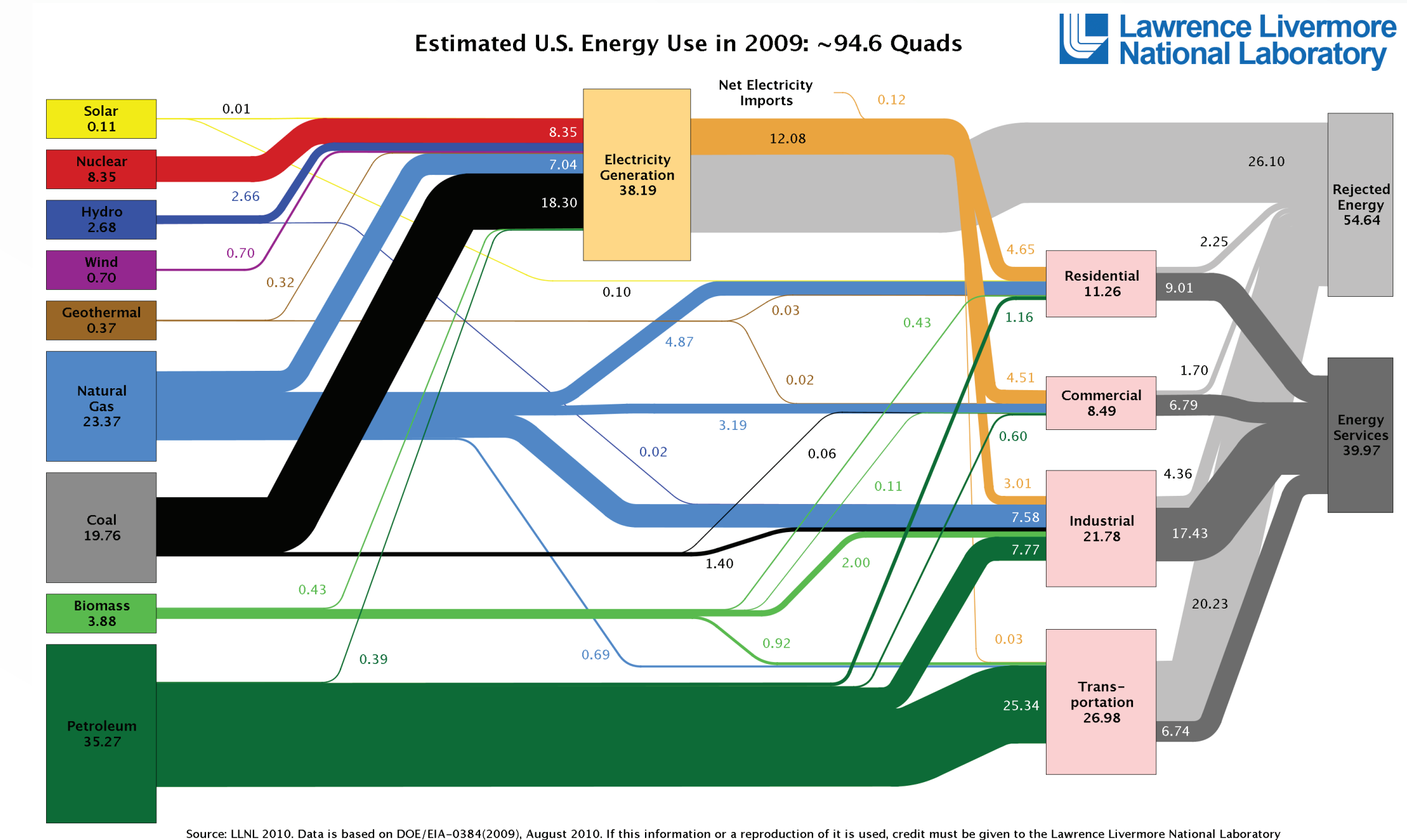


Figure 2: Sankey diagram for 2009 energy usage
LLNL.gov Energy Flow Charts

According to 2009 data, 58 percent of all energy produced and purchased in the US is wasted. Most of this waste heat radiates into the atmosphere and does no good for society. The focus of our work is the efficient harvesting of this and other heat sources with thermoelectric devices.

Thermoelectrics: What they do and how they work

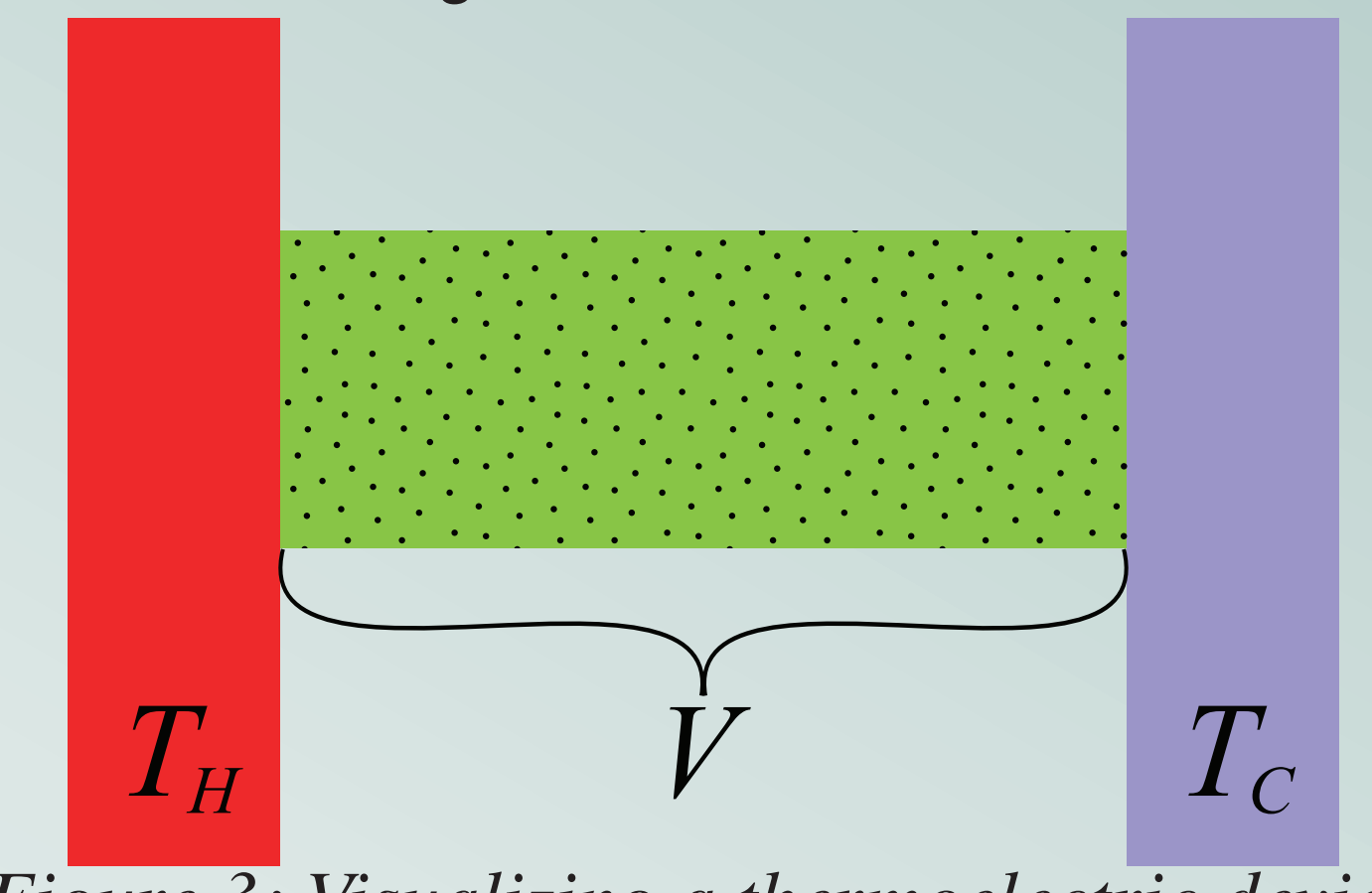


Figure 3: Visualizing a thermoelectric device

Thermoelectrics are devices which exert an electric potential when in the presence of a temperature gradient. The thermoelectric figure of merit, ZT, characterizes the efficiency and viability of a material as a thermoelectric device:

$$ZT = \frac{S^2 \sigma T}{\kappa_{el} + \kappa_{ph}}$$

where S is the Seebeck coefficient, σ represents the material's electrical conductivity, T is temperature, and κ_{el} and κ_{ph} are the electron and phonon thermal conductivities, respectively.

According to the Wiedemann-Franz law, κ_{el} is higher in materials with high σ . Therefore, we must minimize κ_{ph} if we seek to maximize ZT.

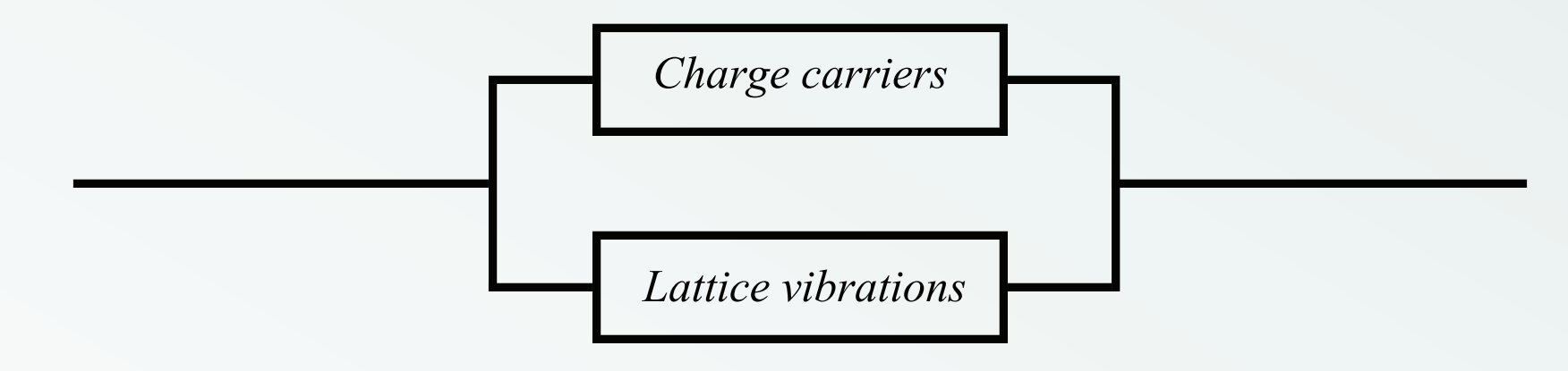


Figure 4: Charge carriers and lattice vibrations are parallel means of energy dissipation.

Our task is to find or create a material with the greatest ZT possible. To this end, we exploit different tools for the exploration of phonon thermal conductivity and thermoelectric properties in general.

Molecular dynamics simulation:

Molecular dynamics is a type of computer simulation which allows the scientist to define the initial state and interaction forces in a system, and study its time evolution. From a philosophical perspective, these programs perform a very simple task: the repeated time integration of Newton's second law of motion.

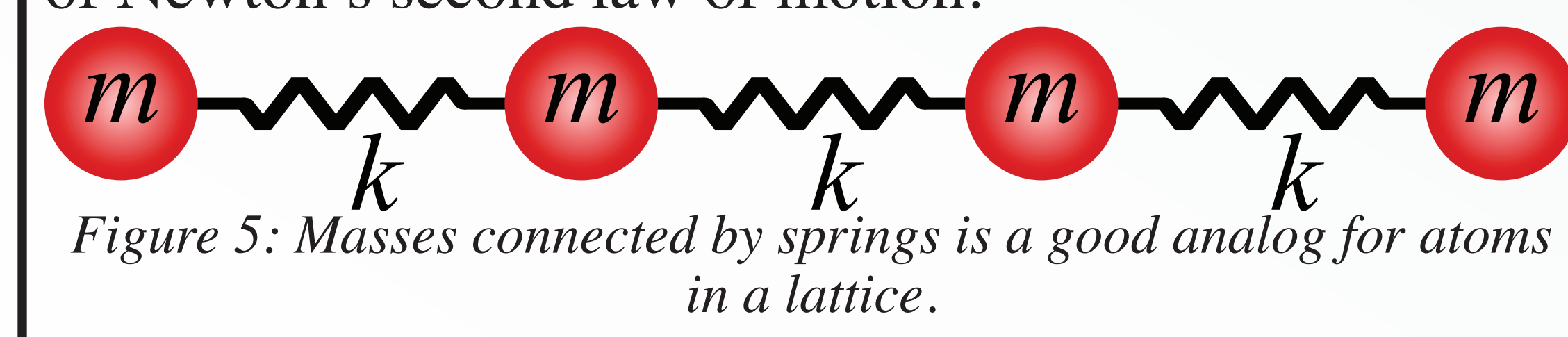


Figure 5: Masses connected by springs is a good analog for atoms in a lattice.

However, this task can prove time consuming especially as system size grows. For this reason, we exploit high performance computing resources.

Our MD simulator of choice is called LAMMPS (Large Atomic/Molecular Massively Parallel Simulator), which is very well suited to running on massively parallel computers by design.



Figure 6: Kraken computer, for whose time we were given a grant

We have employed two means of measuring thermal conductivity of a system in simulation thus far. In the first, different wavepackets are sent down a long, pure lattice which is joined with the material of interest. The wavepacket scatters off the interface, and the amplitude of the transmitted energy is measured at several points in time. From this we can calculate the mean free path, which is related to thermal conductivity.

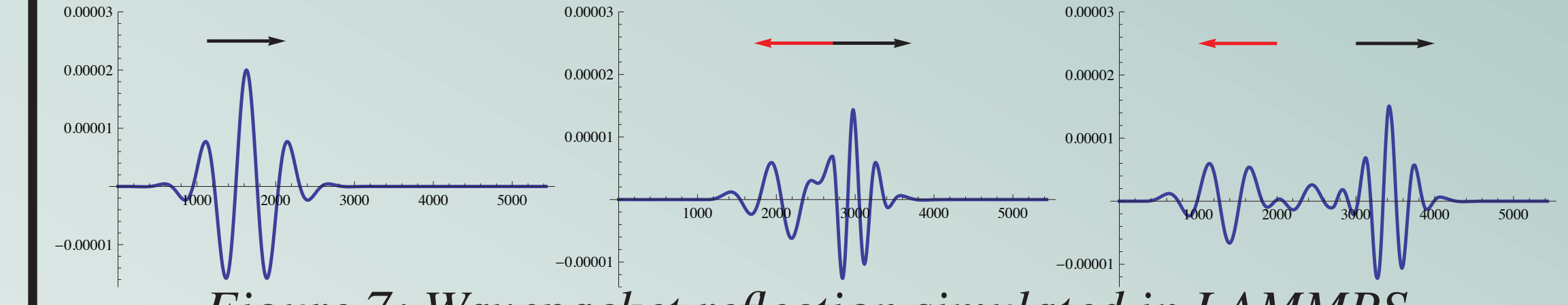


Figure 7: Wavepacket reflection simulated in LAMMPS

The second method of measurement involves the movement of energy from the ends of a system to the middle (typically, periodic boundary conditions are imposed). The simulator will periodically choose the coldest atoms from the center and switch them with the hottest at the ends. This energy flux is increasingly constant in time. In response to the imposed end temperatures, the atoms' energies will form a linear temperature distribution after a long time. Noting the slope of this distribution and the magnitude of average energy flux, thermal conductivity can be calculated for the system.

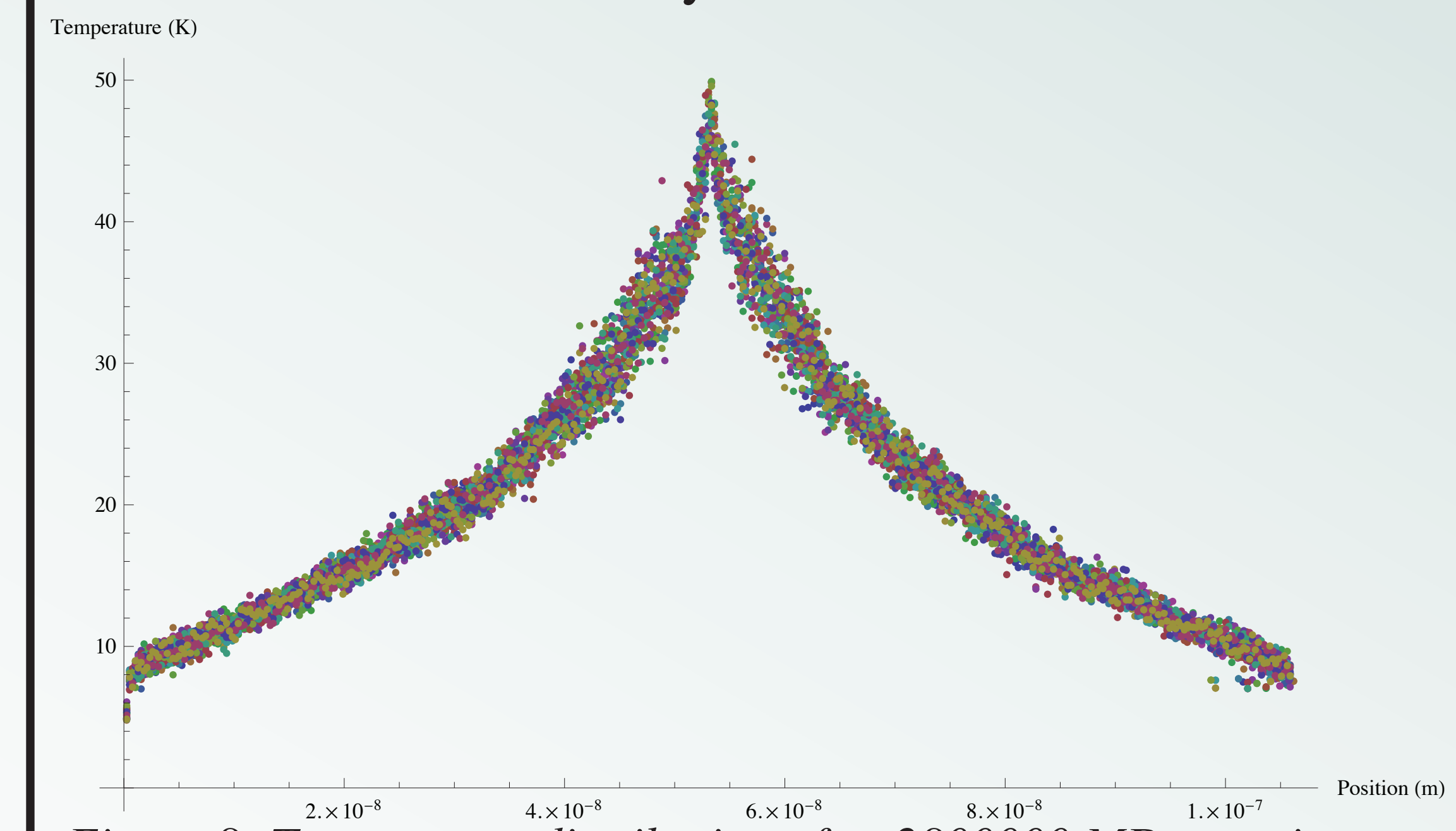


Figure 8: Temperature distribution after 2800000 MD steps in pure sample (reference case)

Build it downstairs:

Once found, an interesting system can be constructed in the lab. Sputtering multilayered structures creates a one dimensional system which we hope will behave as simulation predicts. Our project is only beginning to achieve lab construction and measurement; we have no data of that sort to present at this time. One sample was built, though it could not be measured.

Results:

One of our ideas which generated interesting results involved introducing entire planes of atoms with much greater relative mass. These planes were selected at random throughout the sample. A region in the center of these heavy planes was then assigned to the lighter mass, hoping to further decouple phonon and electron modes.

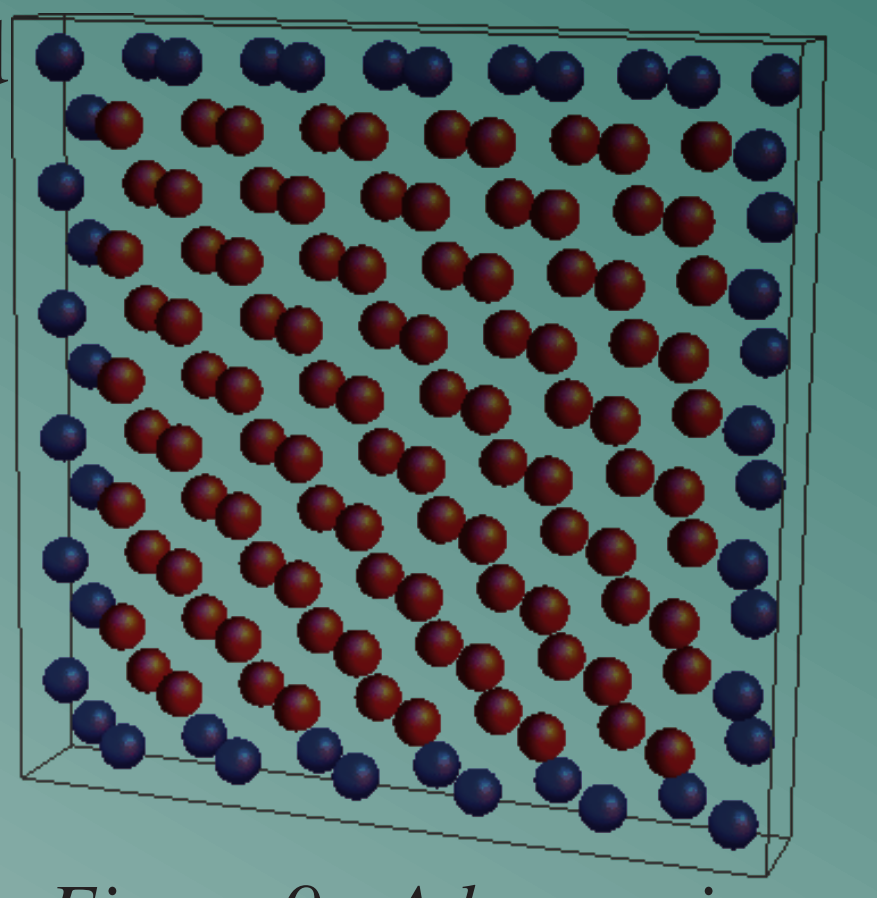


Figure 9: A heavy ring encloses selected planes of atoms

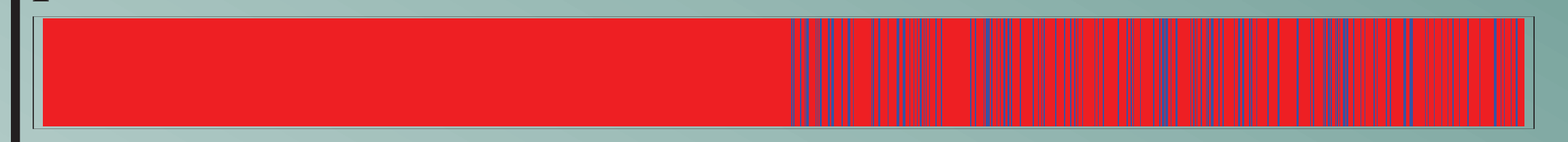


Figure 10: Pictorial representation of disordered lattice

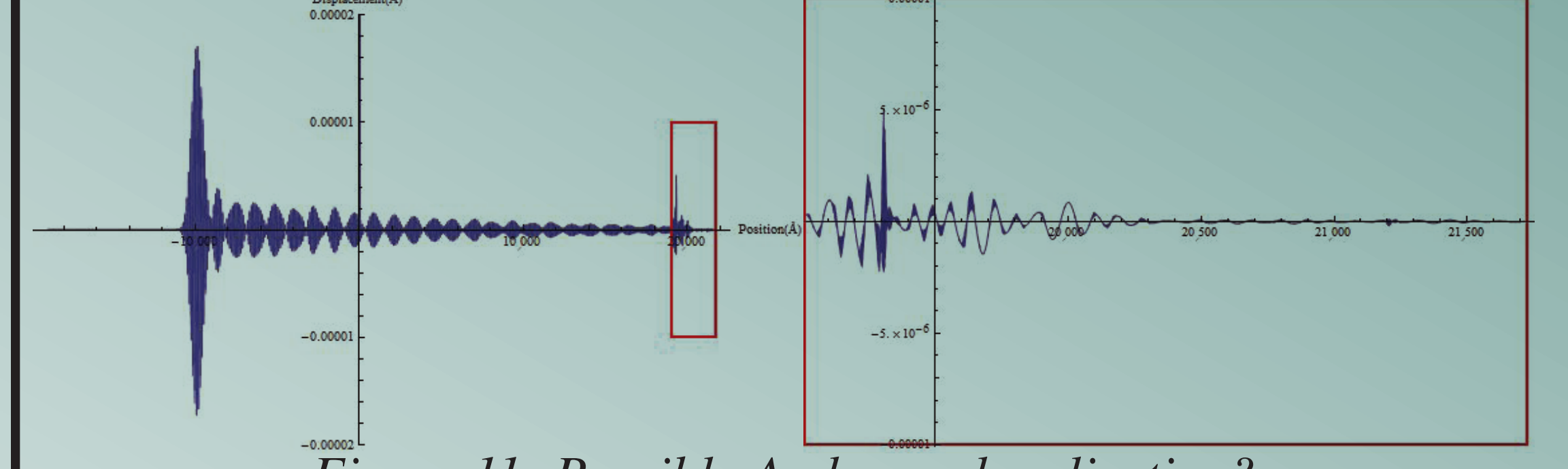


Figure 11: Possible Anderson localization?

The hole was very effective in reflecting incident energy and demonstrated what could be Anderson localization in the region of disorder.

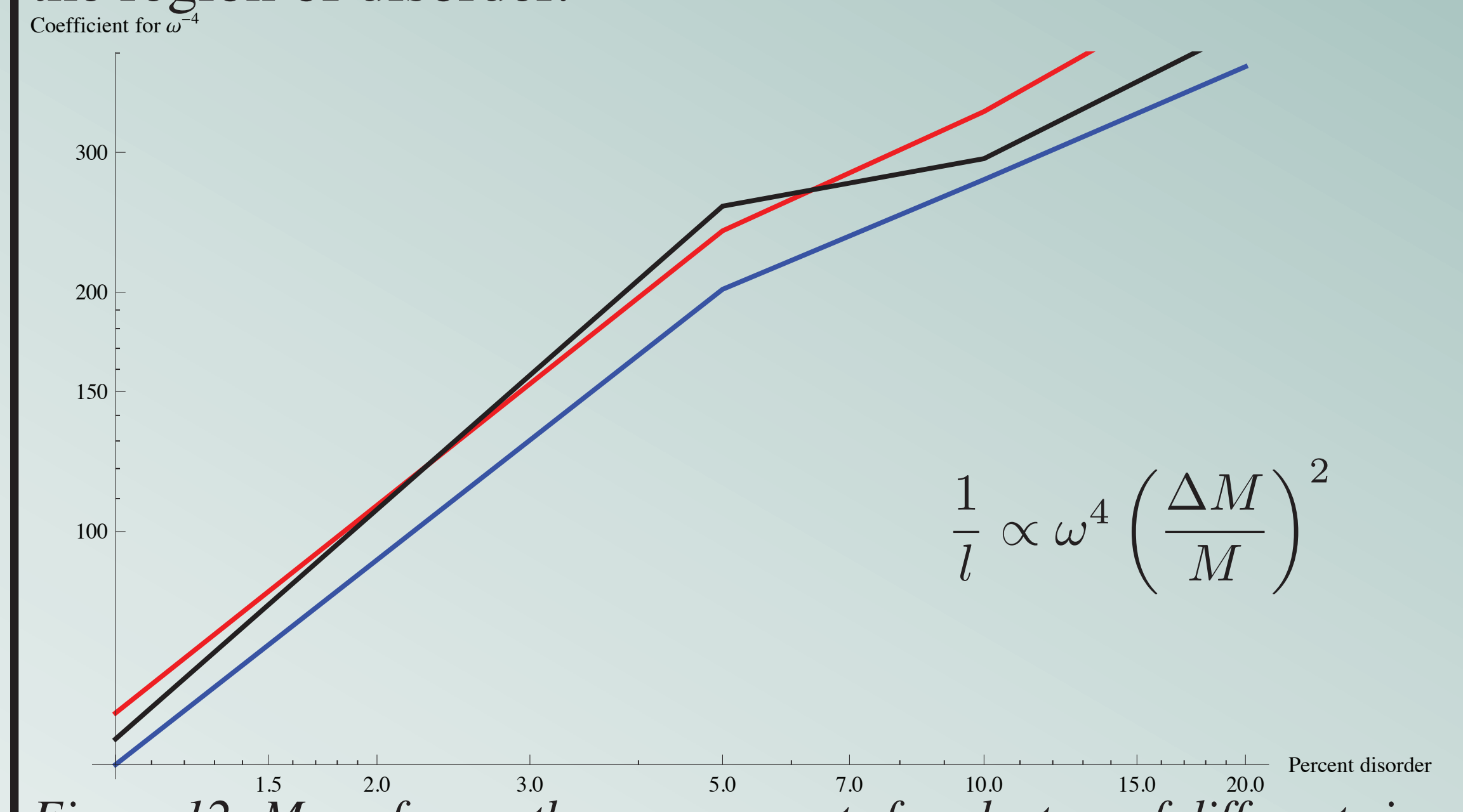


Figure 12: Mean free path measurements for clusters of different sizes (blue is single-atom, red is two-atom, and black is three-atom)

We also tried increasing the mass of atoms in clusters of varying sizes. Though increasing cluster size did decrease phonon mean free path, this effect was small in magnitude.

References:

We gratefully acknowledge support from the Petroleum Research Fund, the Center for Advanced Microelectronic Manufacturing at Binghamton University, and NASA for their support of this work.
S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995). See <http://lammps.sandia.gov>
This research was supported in part by the National Science Foundation through TeraGrid resources provided by NICS under grant number TG-PHY100034