Simulating Meteor Ablation using Molecular Dynamics

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Abstract

Billions of small meteoroids enter the Earth's atmosphere each day, the majority smaller than a milligram. As these particles travel through the atmosphere, they collide with atmospheric molecules that impart energy to the meteoroid. The meteoroids heat up, and sputter off mass and ablate. While there are theories about the heating mechanisms and mass loss of a meteoroid during atmospheric transit, little is known about the in-depth molecular dynamics during the intense heating on the microscale of single particle interactions.

This poster presents molecular dynamics simulations of particle sputtering and heating. We model the physics of atmospheric molecules impacting different meteoroid materials on the atomic scale. The simulations calculate the dynamics of such processes in full 3D, allowing a range of parameters for the impacting molecule and meteoroid lattice energies.

The sputtering yield's dependence on velocity was found to have a different shape than the standard theory predicts. The kinetic energy of the sputtered particles can be described by an inverse gamma distribution, and the thermal energy fraction of impact was found to have a linear relationship when compared to velocity. Most models assume an energy transfer coefficient of unity, whereas these simulations show it is less than one and velocity dependent.

Background

Meteor Ablation:

There are two main processes that contribute to mass loss of a meteoroid due to impact of atmospheric molecules: **thermal ablation (sublimation)** and **sputtering**. While thermal ablation is the main driver of meteoroid mass loss, sputtering does significantly contribute to the mass loss of miniscule meteors on the scale of 10 *ng* and lighter. Sputtering Yield is defined as the number of atoms that overcome the surface potential barrier, and escape the meteoroid[1].

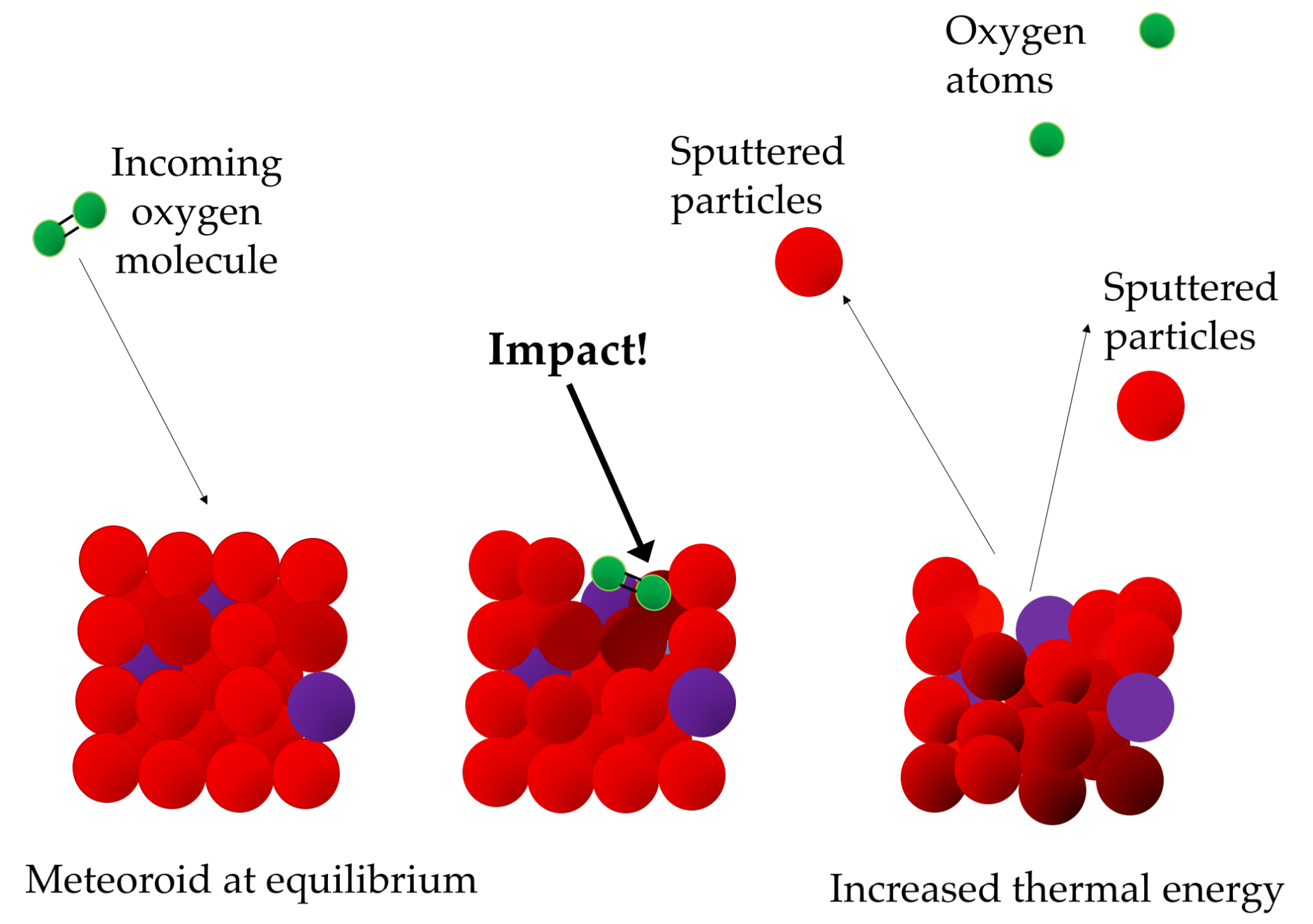


Figure 1. Diagram of impact of Oxygen molecule on lattice of Iron (red) and Nickel (purple) resulting in two sputtered particles

Motivations:

1) How is energy transferred to a meteoroid by the atmospheric molecules?
2) What are the properties of the particles entering the atmosphere?
3) How do these results affect:

i. Interpretation of meteor radar data

Radars observe **head echoes**, reflections from the high density plasma formed by sputtered and ablated particles that collide with atmospheric molecules. Radars cannot directly observe the meteoroid or the the sputtered particles, just their effects on the surrounding atmospheric molecules.

ii. Metal content in the atmosphere

Meteoroid ablation deposits atoms and molecules to the atmosphere. By calculating more accurate ablation yields and energy transfer rates, predictions about meteoric material deposition can be improved.

iii. Meteoroid simulations and models

There are simulations to model the creation of the **meteor plasma,** but they rely on a simple model of meteor ablation. Better understanding of ablation will improve initial conditions for meteor. models and simulations.

Meteoroids:

Four different types of meteoroids will be used as targets, representing both meteoric **iron, stony** chondrites, and achondrite meteors. It is a simplification to use 100% of the same material to build meteoroids, but the scale of the simulation is small enough that it is be appropriate to approximate a uniform composition for an area of impact[3].

	Meteoric Iron	Stony: Crystalized	Stony: Amorphous	Stony: Carbonaceous
Material	Iron-Nickel Alloy	Quartz	Amorphous Silica	Moissanite
Composition	$Fe^{0.9}Ni^{0.1}$	SiO_4	SiO_2	SiC
Density [g/cc]	7.5-8	2.5-3.5	1.5-2.5	3-3.5
Origin	Asteroid core	Asteroid crust	Asteroid crust	Asteroid crust
Crystal	BCC	Trigonal	Non-crystalline	Hexagonal

Table 1: Table of target meteoroid properties

Methodology

Simulation Overview:

These molecular dynamics simulations are performed using LAMMPS, the Large-scale Atomic/Molecular Massively Parallel Simulator[2]. The idea is to create an equilibrium lattice structure at 0 *K* and warm it slowly to the desired temperature, which is 250 *K*. The meteoroid is then exposed to vacuum on one side and allowed to equilibrate again. The equilibrium state is saved and a single atmospheric molecule is made to impact the lattice travelling at meteoric velocities (11-72 *km/s*). The energy, temperature, and the number of sputtered atoms are recorded and analyzed.

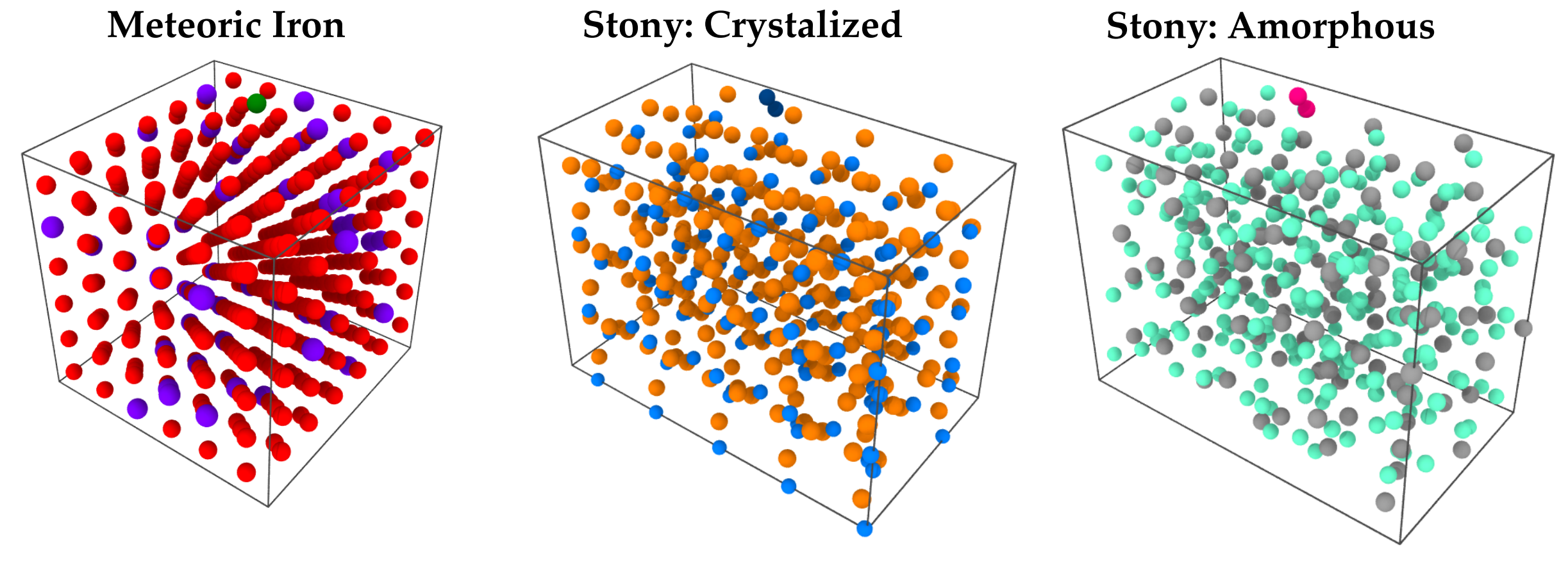


Figure 2: Iron-Nickel, Crystalized SiO_2, and Amorphous SiO_2 lattices (from left to right) with oxygen molecule right before impact

Results

Sputtering Yield:

The simulation was run with 256 times for each of the five different impact velocities (23.2, 35.4, 47.6, 59.8, and 72.0 *km/s*), with all the molecules impacting at normal incidence. The difference in the number of atoms at the start and end of the simulation were used to calculate the sputtering yield in the plots on the right (Fig. 3). The simulated yield is close to the theory[4] but does have a different shape. The discrepancy may be due to the theory assuming charged, single particle impactors instead of neutral atoms/molecules.

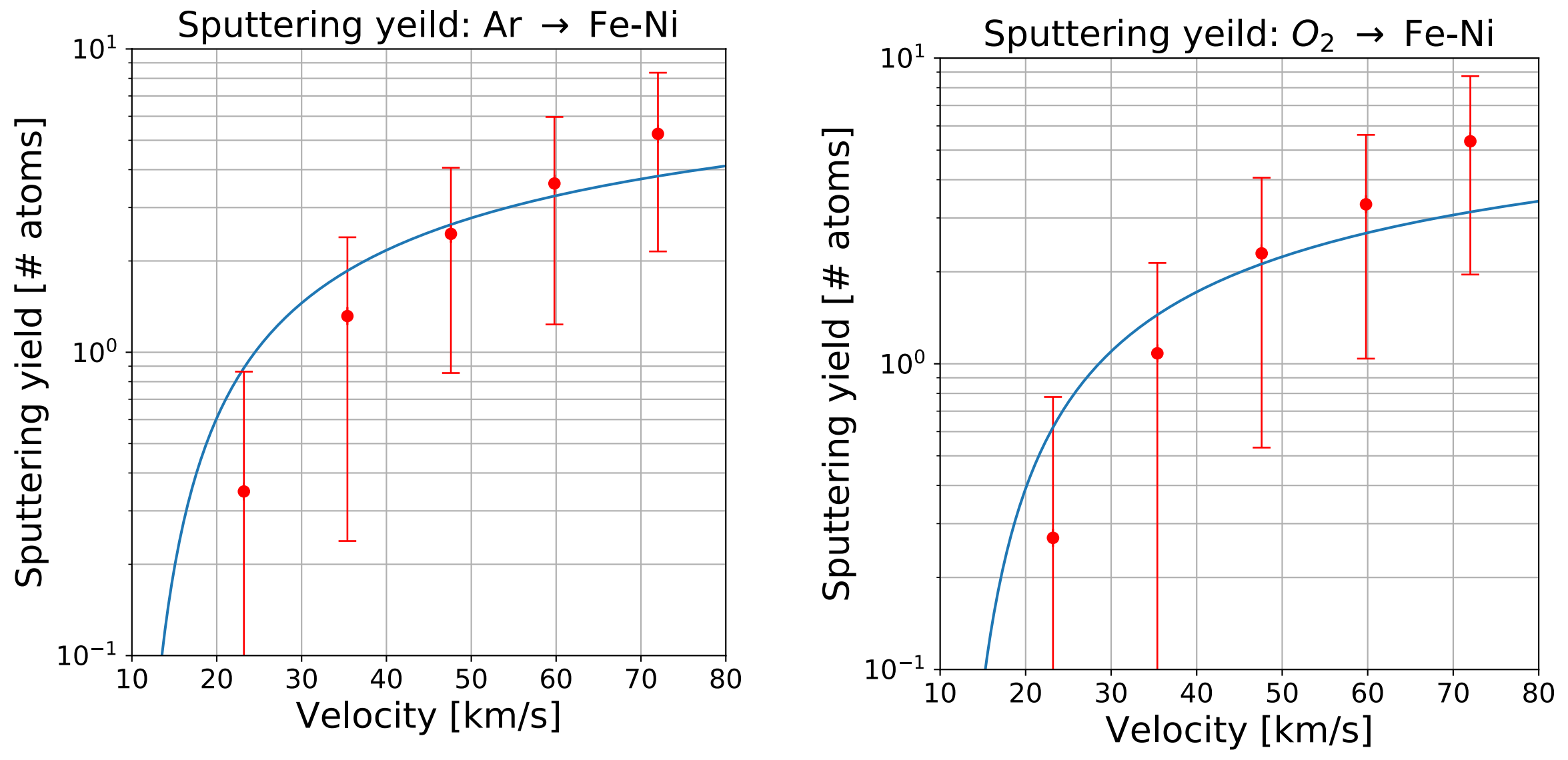


Figure 3: Yield as a function of impact particle type and velocity, as well as target composition. Simulations in red, theory in blue.

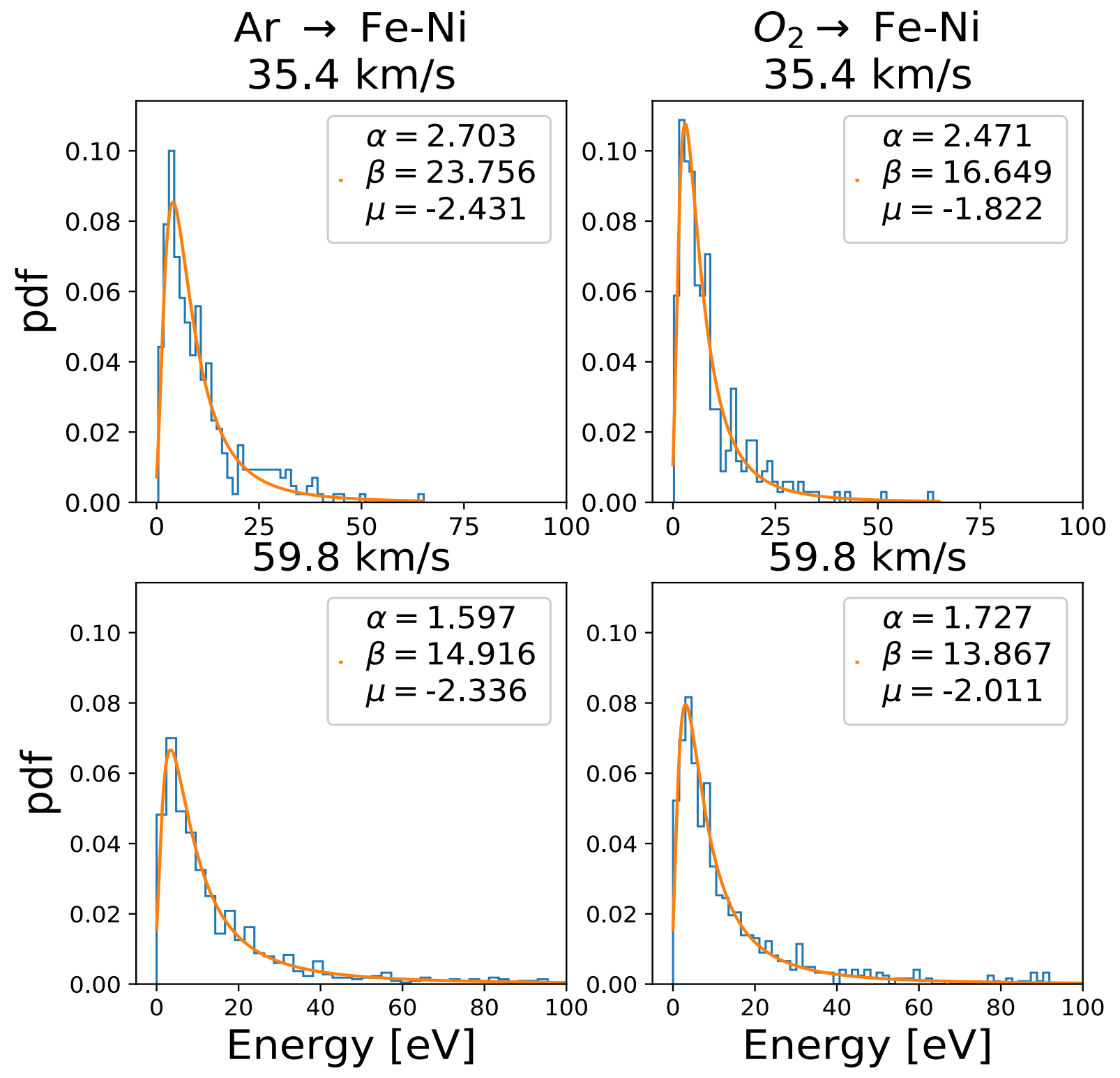


Figure 4: Energy histograms for sputtered particles.

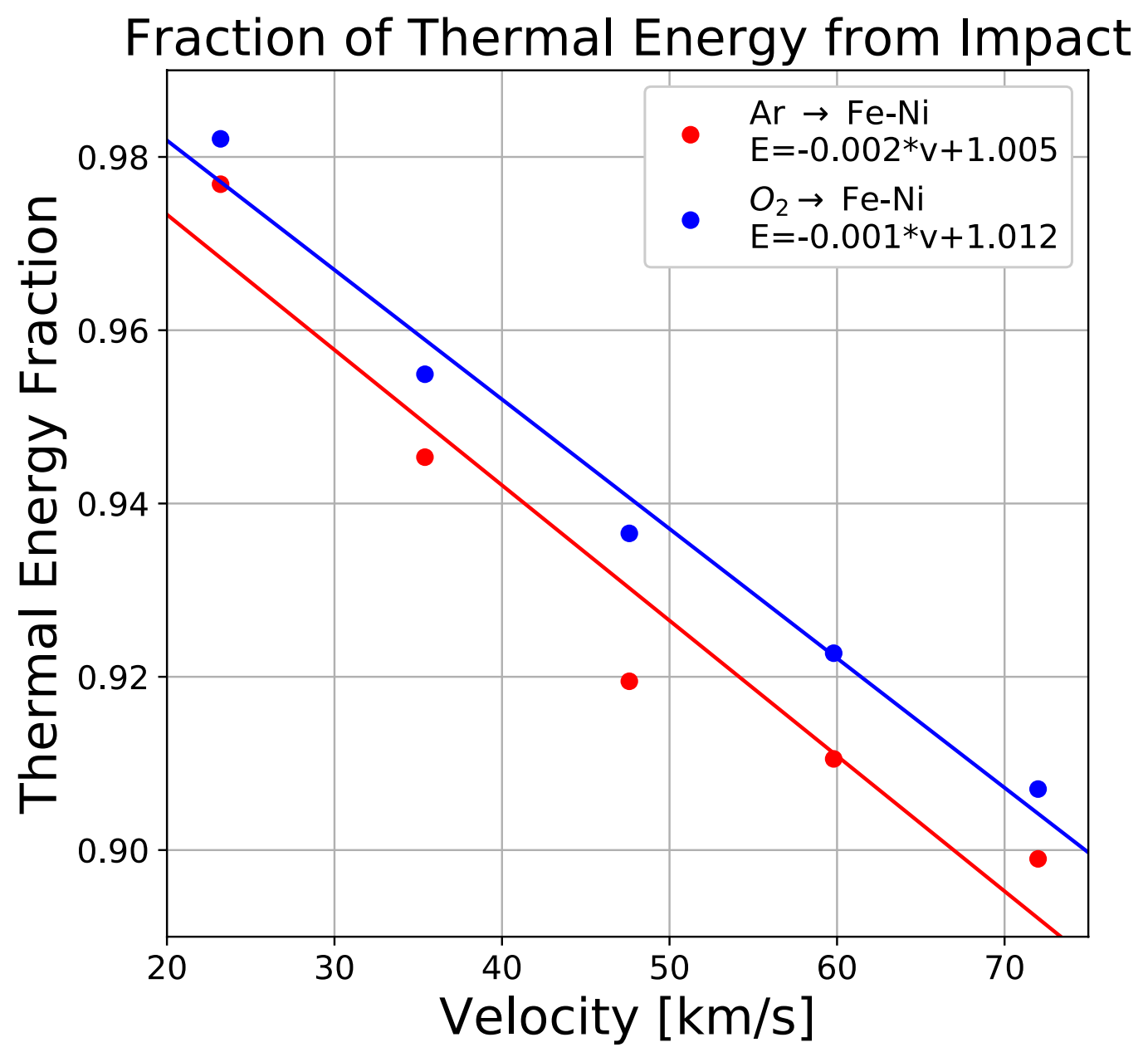


Figure 5: Energy transferred to the meteoroid.

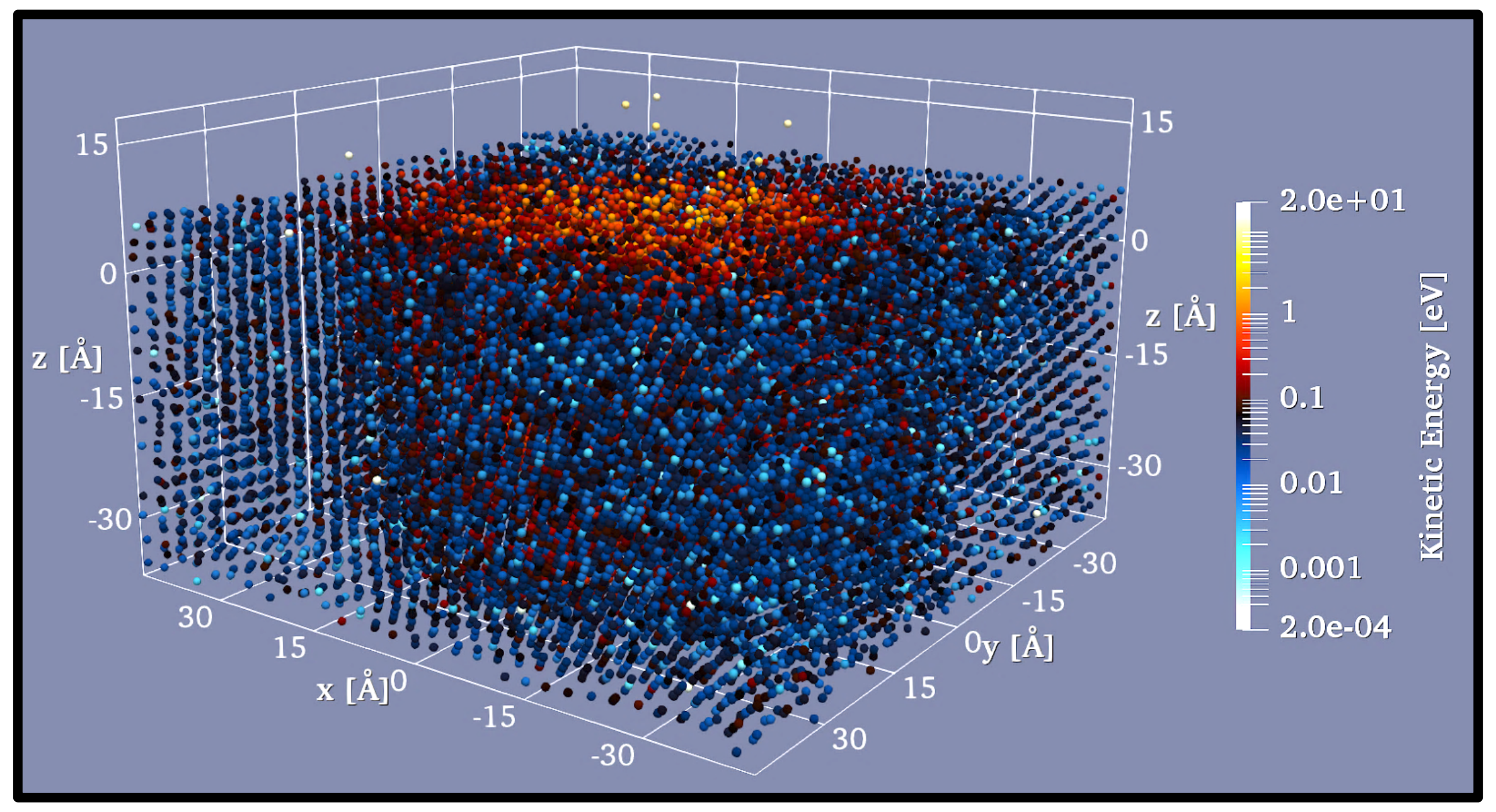
Energy Transfer:

We use the change in total energy as sputtered atoms leave the simulation as a method of monitoring energy loss. There are two example probability distributions of sputtered particles energy to the left (Fig. 4), with impact velocities of 35.4 and 59.8 *km/s*, fit with an inverse gamma distribution. These can be used for more realistic energy distributions in meteor plasma simulations

By comparing the total energy of the sputtered particle to the energy of the impacting particle, the thermal energy fraction coefficient as a function of velocity and impactor type is calculated and shown to the left (Fig. 5). There is a linear relation between the velocity and thermal energy fraction, as opposed to the assumption of unity across all velocities used in meteor modeling. A transfer coefficient less than one means that meteors burn up less rapidly than models predict.

After the impact, the energy transferred to the meteoroid spreads. This is seen in Fig. 6, which shows the kinetic energy of individual atoms in the meteroroid near the impact site at the *(x,y) = (0,0)*. The rate of heating through the meteoroid can change the way meteoroid models apply heating to a non uniform scale.

Figure 6: 3D model of iron-nickel lattice after impact. The color is kinetic energy of individual atoms. Sputtered atoms, with large kinetic energy are visible above the meteoroid.



Conclusion

Molecular dynamics allows for in depth analysis of meteoroid ablation on the atomic scale. The sputtering yield differs from the yield projected by the theory in [4]. The distribution of kinetic energy of sputtered atoms was found to nicely fit an inverse gamma function, and the thermal energy imparted to the lattice was found to have a linear relationship to impact velocity. Future work includes expanding the simulations to more target materials and more impacting atoms, as well varying impact angle. The simulated results will replace assumptions inherent in ablation models. Ultimately, we will apply these microscopic simulations to improve macroscopic data analysis, theory, and simulations.

References

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Further Information

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