Hydrogen Collision Dynamics on a Rough Nickel Surface

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Abstract— **Three frames from a molecular dynamics video which depicts the interaction of a 10-eV hydrogen atom with a rough nickel surface at 300 K are shown. The potential energy and velocity vectors of all the atoms are shown through imaginative graphics. A reflection, an absorption, and a re-entrant flight are shown.**

I. Simulation

THE interaction of a 10-eV hydrogen atom impacting on a rough nickel surface was simulated using the molecular dynamics code Dyn52 [1]. The surface consisted of six by six face-centered cubic unit cells, eight unit cells deep, and a surface feature consisting of a four-sided pyramid of atoms with an additional atom in the center of each of the four faces. There was also a small pyramid of only five atoms off to one side. The 0.5-fs time-step was chosen so the incident atoms would travel much less than one lattice spacing per step. Eleven different runs of 200 to 1200 time-steps each were conducted. On an Cray XMP-48, each time-step took approximately 8.5 CPU seconds. The positions, energies, and velocities of each of the 1048 nickel atoms and the hydrogen atom were recorded at each step. Each atom interacted with all other atoms in the simulation, though only the nearest 15 or so neighbors to the incident hydrogen atom were significant.

Three of the runs were chosen for visualization and have been published [2] as a "video book" complete with a technical explanation, references, and advanced graphics. These runs showed a reflection, an absorption, and a re-entrant flight where the atom left the surface, but with insufficient velocity to escape the effect of the surface potential and was drawn back to the surface by the presence of atoms in the surface feature. Many other effects are observable in the video and discussed in the video book.

In the video and the figures shown here, the nickel lattice continues below the atoms shown in the negative z (downward) direction. Shadows of the atoms are shown on walls and a floor placed behind and below the lattice for visual clarity. The potential energy of each atom in the lattice is given by its color. All the nickel atoms are bound and have a negative potential energy ranging from approximately -2 to -4 eV. To visualize the flight of the incident hydrogen atom more easily the visual size of the atoms in the lattice were reduced and a yellow tube was left along the path taken by the hydrogen atom. To show the resulting motion of the lattice atoms, each sphere was given an arrow head which points in the direction of motion for the atom. The length of the arrow indicates the atoms' speed. Initially, these vectors point in random directions due to the 300 K thermal energy. The base of the vectors represent the lattice atom's positions. While the actual positions of the atoms, and thus the base of the arrows are moving, their movement is much too slow to be seen in the time-scale of these simulations. The acceleration and thus the force on each atom can be seen clearly by watching the change in direction and color of the velocity vector.

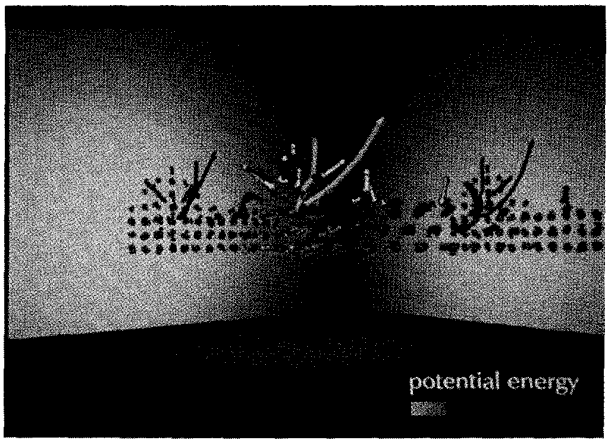

Fig. 1. Reflection of a 10-eV hydrogen atom from nickel.

A Silicon Graphics 240 GTX computer was used to render the computer graphics using Wavefront® and additional software developed by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. Approximately 5000 individual frames were rendered for this project. Each frame took between 1 and 15 min of CPU time to complete. The video lasts 37 min. Approximately one hour of production time was needed for each minute of video to combine the rendered frames, narration, and superposition of graphics and live action.

II. Results

Fig. 1 shows the reflection of the 10-eV hydrogen atom from the lattice. It underwent two hard binary collisions which changed the momentary potential energy of those lattice atoms by 2 eV, and several softer nonbinary collisions. The collisions are primarily elastic though, and the hydrogen atoms emerge from the lattice with 8.5 eV of energy. Even the two hardest hit nickel atoms return to thermal energies within 40 fs.

In the second simulation, the hydrogen atom penetrates a few atomic layers and then travels horizontally just below the surface for 18 Å. At that point, the hydrogen atom is knocked downward and never resurfaces. Fig. 2 shows a close-up frame from the start of the run. The yellow atom on the right is one of the binary-collision partners involved in a hard direction-changing collisions. In the video book, this flight is compared favorably to a fractal TRIM simulation [3] in terms of the

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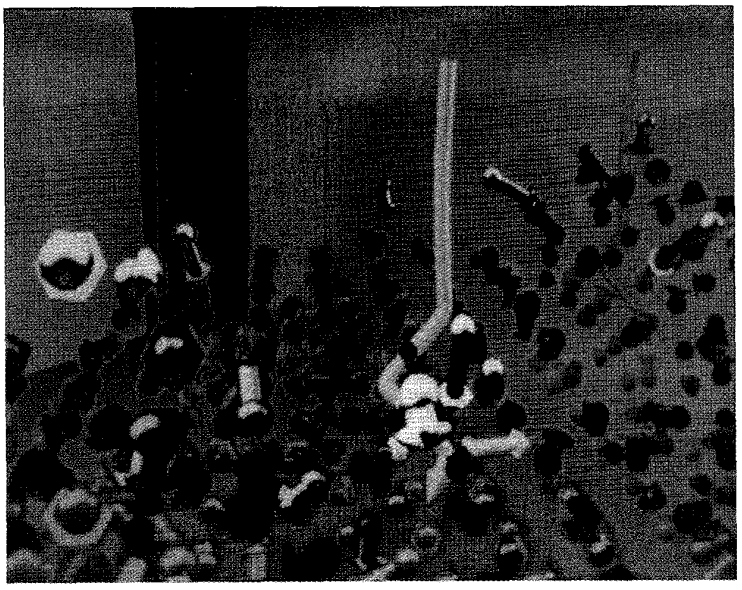

Fig. 2. A binary collision during the reflection process.

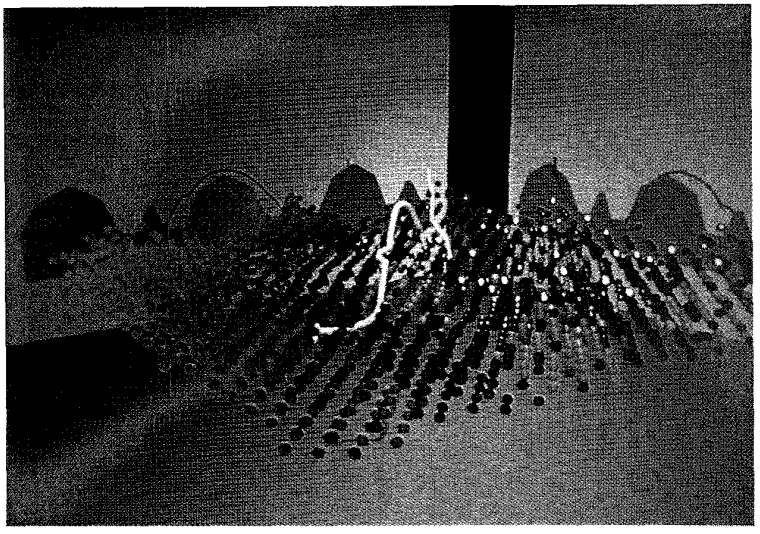

Fig. 3. The end of the re-entrant flight.

average distance between binary collision and the number of binary collisions that occur.

The third simulation details several ion–surface interactions. These include the effects of surface roughness, interference of shock patterns from hard collisions, visual proof of the work function concept, a mechanism by which particles can come quickly to rest, and a possible explanation of below-threshold sputtering. Fig. 3 shows one frame near the end of the flight. The hydrogen atom entered the surface, had three rapid interactions—the first and third with the same atom—and was propelled outward skimming the surface feature. It did not have enough energy to escape the surface potential and traveled back down the other side of the feature. Upon impacting the surface, the atom quickly came to rest imparting several electronvolts to the lattice spread among two or three neighboring atoms.

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REFERENCES

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