Electronic Stopping of slow H and He in gold from first principles

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Outline of this talk

- Electronic stopping power
- Electronic stopping in Jellium
- Electronic stopping in metals: simple vs transition metals
- Our TDDFT calculations on gold using SIESTA
Electronic Stopping Power

- A charged particle moving through a solid material interacts with it and loses its kinetic energy to both the electrons and the nuclei inside it.
- Amount of energy given to electrons per unit distance is called electronic stopping power.
Electronic stopping in Jellium

• For a slow moving projectile, the electronic stopping is proportional to the velocity of the projectile.

• The proportionality constant depends on the projectile and the density of electrons in the jellium.
What do Experiments find?

Do metals act like a jellium?

- Sp-bonded metals, e.g., Al: $S \sim v$

- Transition metals, e.g., Cu: slope increases around $v = 0.1 - 0.2$ a.u.
An Example: H and He in gold

\[ \varepsilon = S/n_a \]

\[ r_s \sim 1/n^{1/3} \]

..., 5d\textsuperscript{10}, 6s\textsuperscript{1}

DFT: Echenique et al.
Solid State Communications, 37, 779 (1981)
Our calculations

• Ehrenfest Dynamics

• Electrons - Quantum Mechanics
  Time Dependent Density Functional Theory

• Ions - Classical Mechanics
Results

Simulations (this work, <100> channel)
- ● He
- ○ H

Experiments
Figueroa et al. (<100> channel)
- H

Markin et al. (polycrystalline)
- ★ He
- ○ H
Condor Script

Universe = standard
Executable = /home/maz24/siesta-25april11
Input = AuH.fdf
transfer_input_files = Au.psf,H.psf,AuH.XVi,AuH.VERLET_RESTARTi,AuH.DM,
AuH.TDWF,AuH.etot_vs_time
should_transfer_files = YES
when_to_transfer_output = ON_EXIT_OR_EVICT
Requirements = OpSys == "LINUX" && Memory >= 2000 && Arch =="X86_64"
Output = out
Log = logfile
Error = ERR

Initialdir = d005
  Queue

Initialdir = d010
  Queue

Initialdir = d015
  Queue
Electronic distribution in adiabatic states

\[ C_{ij} = \langle \Phi_i^X | \Psi_j^X(t) \rangle \]

\[ O(E) = \sum_{i,j} |C_{ij}|^2 \delta(E - E_i) \]

\[ P(E) = O(E) - \Theta(E_F - E)g(E) \]
H → Au <100>

$\nu = 0.05$ a.u.

$t = 0.1 - 1.1$ fs

$\Delta t = 0.1$ fs

A short transient

$E_F$
Au: $v = 0.1$ a.u.

Au: $v = 0.5$ a.u.

Na (gold lattice)

$r_s = 1.49$

$r_s = 3.04$
Static impurity screening: a change in electronic distribution in adiabatic states without the impurity
Summary & Conclusions

• We obtained a very good quantitative agreement with the experiments. Jellium picture does not fit on transition metals.

• Our method can be used to describe non-adiabatic processes in real materials.
Thanks!