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From Warm Dense Matter to Defects Evolution Under Irradiation

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- 1. Electron-temperature dependent interionic potential for Au
- 2. Picosecond laser ablation of Au
- 3. Radiation damage in Mo

Electron-temperature dependent interionic potential for Au

2T Atomistic Model of Irradiation

- MD for ions + thermostat due to electrons $m\frac{d\vec{v}_i}{dt} = \vec{F}_i - \beta \vec{v}_i + A \vec{\xi} (t)$
- Interionic potential:
- electron temperature dependent (ETD)

- Thermal conductivity equation for electronic subsystem:

$$C_{e} \frac{\partial T_{e}}{\partial t} = \nabla \left(\kappa_{e} \nabla T_{e} \right) - G_{p} \left(T_{e} - T_{a} \right)$$



ETD-potential for Au



Verification of ETD-potential at $T_e = 0.1 \text{ eV}$



	V_0 , Å ³	E _c , eV	C ₁₁ , GPa	C ₁₂ , GPa	T _{melt} , K
experiment	10.22	3.8	202	170	1338
MD	10.23	4.1	225	180	1210

Au isotherms at $T_i = 300$ K and various temperatures T_e 160 120 6 eV P, GPa 80 3 eV_ 40 0.1 eV 0 0.06 0.08

δ 0.07 ρ, ion/Å³

Atomistic simulation of laser ablation of Au

Picosecond laser ablation



2T Atomistic Model of Irradiation Laser pulse





2T Atomistic Model of Irradiation

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$I = 500 J/m^2$

d = 20 nm

Ablation on short and long timescales



Ablation on short and long timescales



 $I = 1600 J/m^2$

Ablation on short and long timescales

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$I = 1600 J/m^2$

Dependence of crater depth on absorbed fluence



Atomistic simulation of radiation damage in Mo

Damage produced by fission products







- primary radiation damage
- clustering of defects
- change of the mechanical properties

Damage produced by fission products: swelling



- • 20% cold-worked 316 stainless steel tube used for fast reactor fuel cladding.
- Irradiated to ~80 dpa at 510°C.
- ~33% increase in volume, leading to linear strains of ~10%.
- Swelling in absence of physical constraints is <u>completely</u> <u>isotropic</u>.
- Constrained swelling leads to stresses that generate anisotropic distribution of strains.

Constructing interatomic potentials for Mo-Mo, Mo-Xe, U-U



EAM potential for Mo that describes energies of defects



Mo irradiation by Xe ions: evolution of defects



Displacement cascade: Self interstitial atom clusters



Displacement cascade: vacancy dislocation loops



(110) Surface 1000 K, 3.16 A E (Xe) = 42 keV 80x60x60 (Starikov Mo-Xe)

Coordination number

Displacement cascade: vacancy dislocation loops

(110) Surface 80x60x60

1000 K, 3.16 A E (Xe) = 42 keV (Starikov Mo-Xe)





Conclusions

1.Electron temperature dependent potential is constructed by force matching to DFT data

2. High electron pressure lead to a faster expansion and ablation at "short" times

3.Dependence of ablation depth on absorbed fluence: self-consistent description of different experiment is achieved

4.Mo foils under Xe irradiation: vacancy dislocation loops formation near the surface

5.Increase of the ion mass lead to an increased of the defect yield