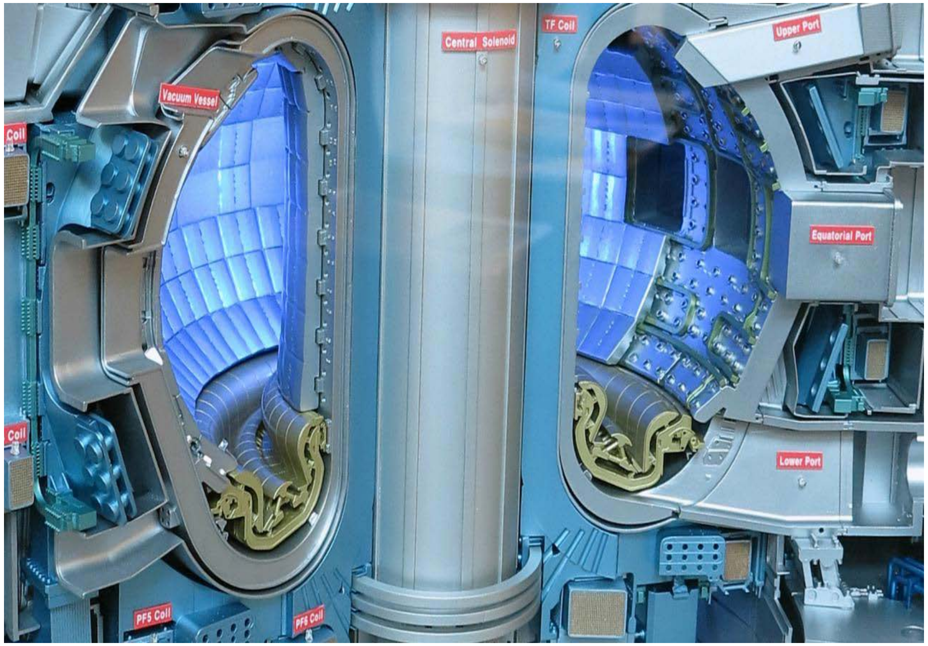
Thermal gradient effect on the helium and intrinsic defects transport properties in Tungsten

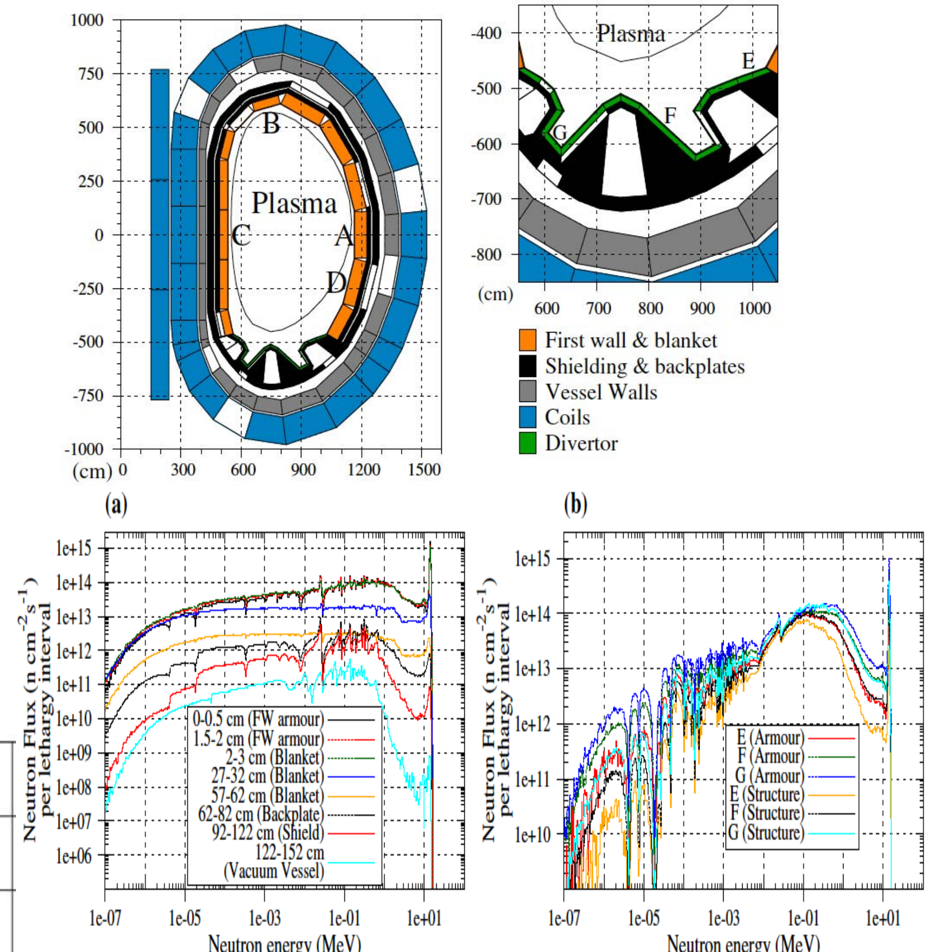
Enrique Martínez
Nithin Mathew
Danny Perez
Dimitrios Maroudas
Brian Wirth

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

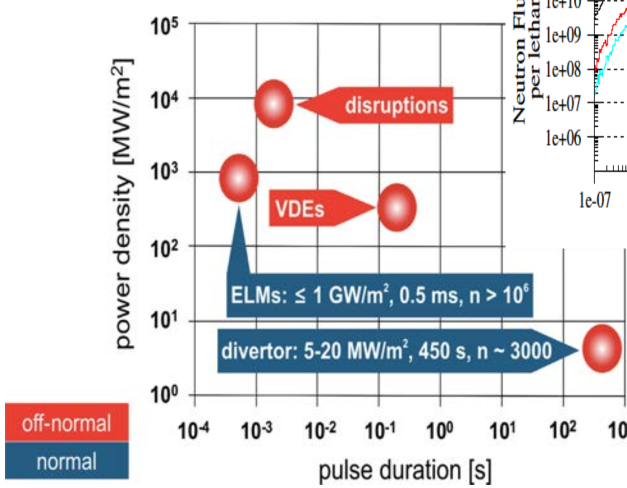
Plasma-Materials Interactions – Materials under Extreme Conditions



Gilbert et al. Nucl. Fusion 52 (2012) 083019



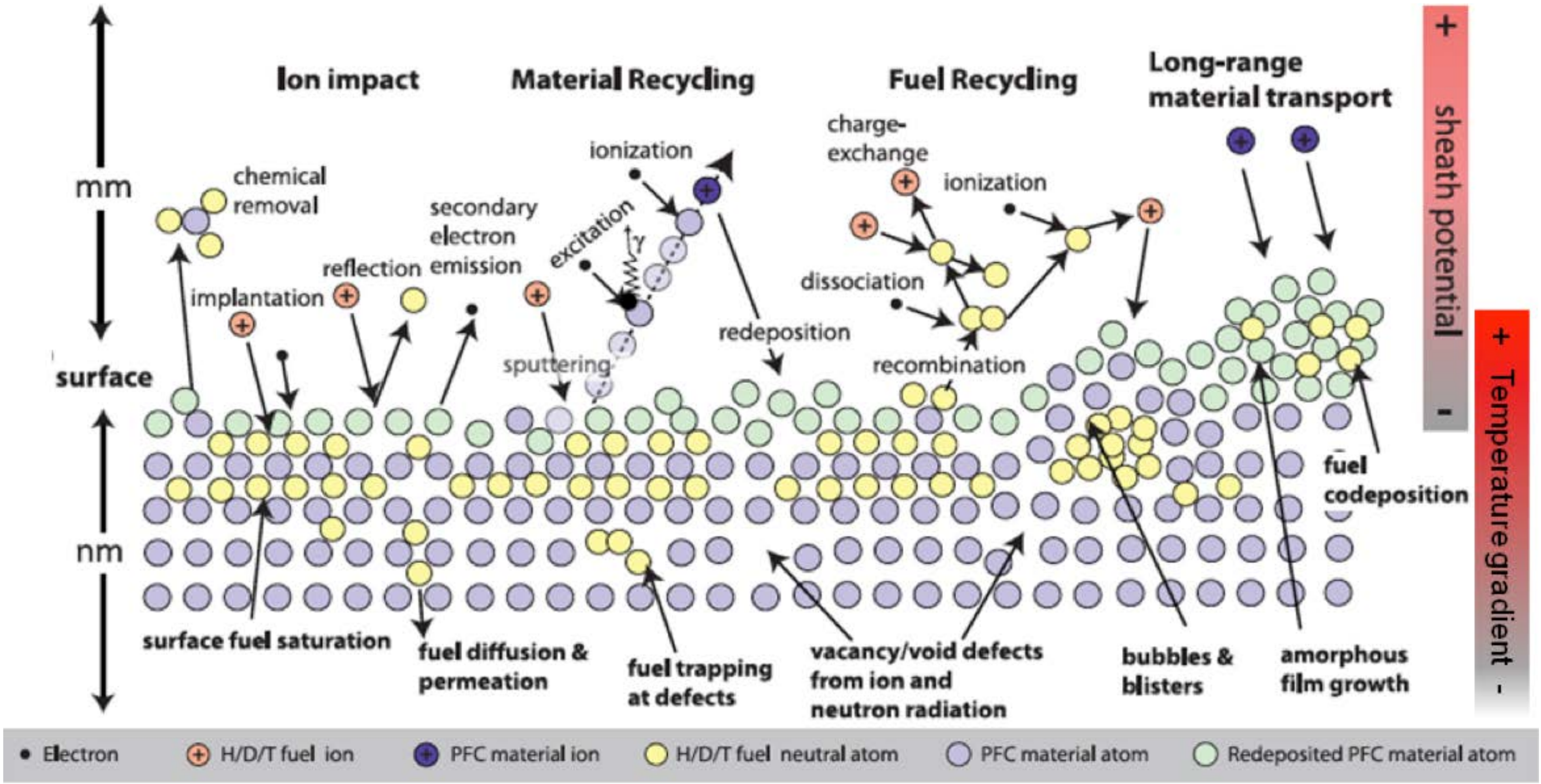
The divertor region will be subject to particle flux (He, D, T, n) and a total heat flux of about 5-20 MW/m^2 to ~10 GW/m^2. These fluxes lead to strong thermal and concentration gradients and changes in morphology that can compromise the integrity of the material.



Spatial overlap between neutron irradiation and plasma particles leads to strong synergistic effects

Plasma Material Interactions

B. Wirth et al. MRS Bulletin 36, 2011



Complex interactions between plasma and the material

Tungsten as PFC Material of Choice

Critical variables

PROS

- High melting temperature.
- High sputter threshold.
- Good heat conduction.
- Small tritium retention.
- Radiation tolerance (compared to austenitic steels).
- High creep resistance.
- Good high-temperature strength.
- Low vapor pressure.
- Low neutron activation.

CONS

- Very low fracture toughness.
- Blistering (<800 K); He bubbles (1250-1600 K); pit, holes and bubbles (1600 K).
- Fuzz formation ?
- Swelling?
- Radiation tolerance (not enough for fusion conditions).
- Transient melting and deformation.
- Low oxidation resistance.
- **Heat flux in transients**.
- High DBTT.

Advanced Designs

Controlled Microstructures

- Ultra-fine and nanocrystalline W
- Additive Manufacturing
- Nano-composites (multilayered materials)

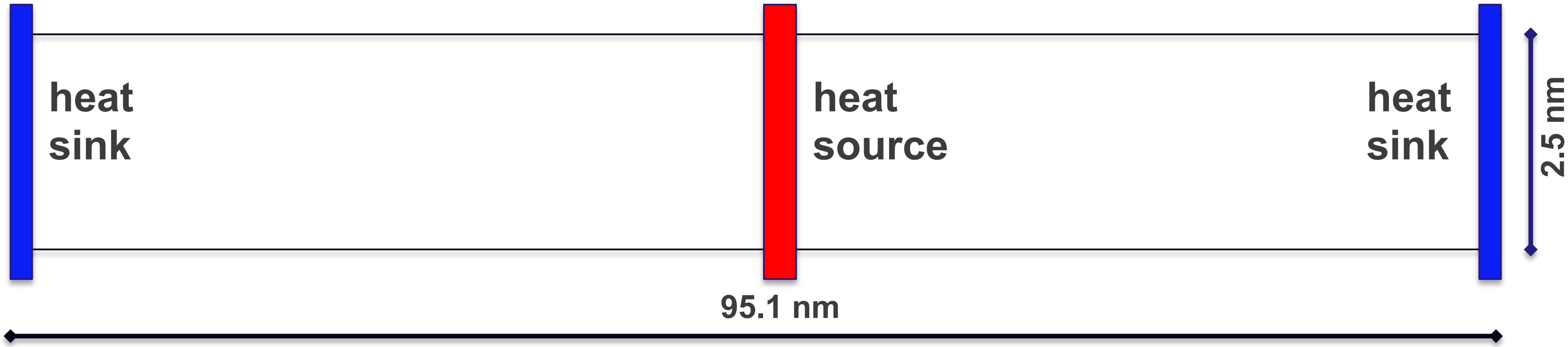
Design variables ⟷

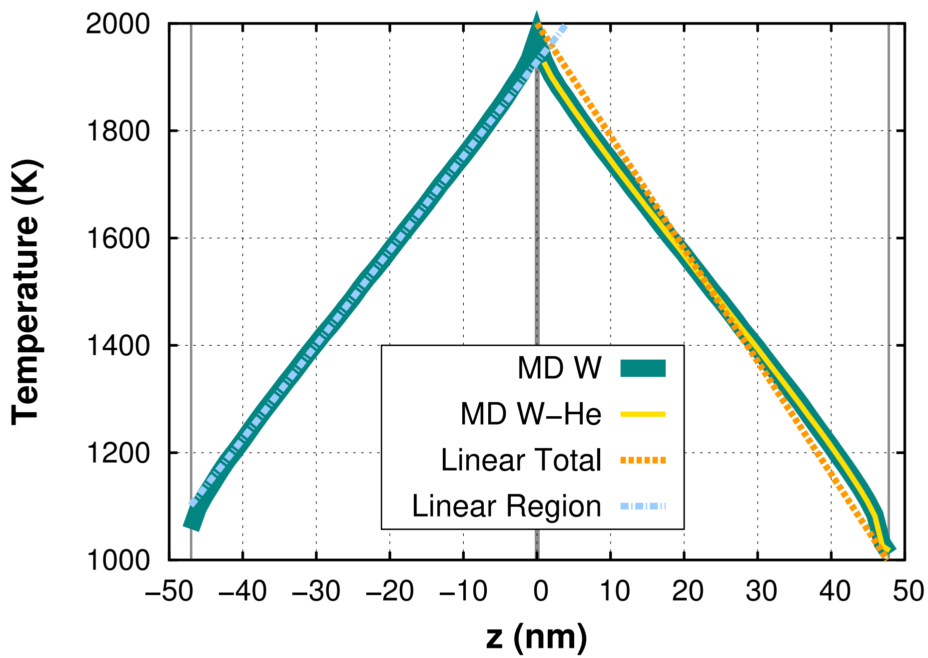
Alloy Composition

- W-X
- High Entropy Alloys
- ODS steels

Computational Methods

- **Non-equilibrium molecular dynamics**





The imposed thermal gradient is 2.1 K/nm (orange line).

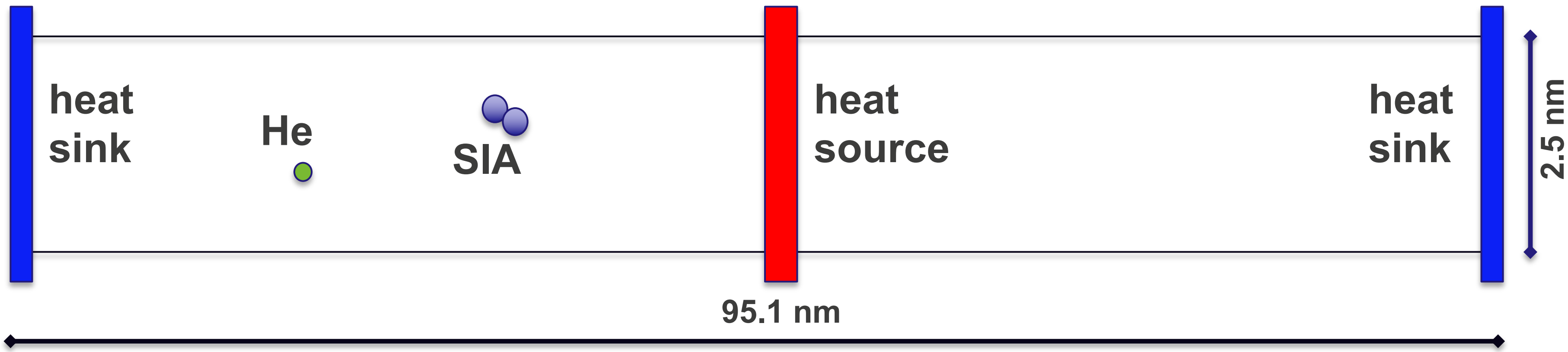
The temperature profile is close to linear with small deviations close to the edges (heat source and sink).

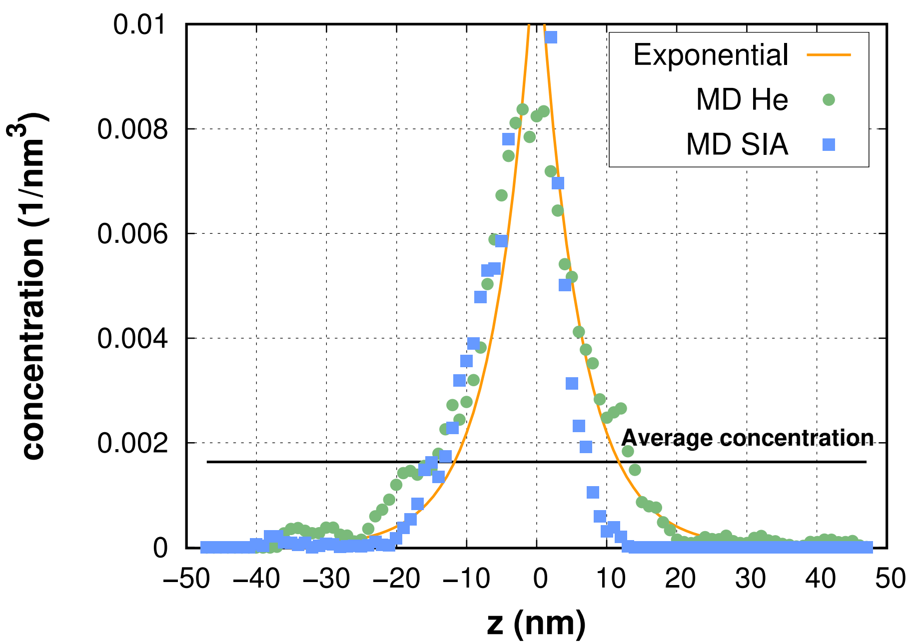
T(z)=2000-2.1z

The fit to the linear region of the temperature profile gives a slope of 1.75 K/nm

Computational Methods

- **Non-equilibrium molecular dynamics**





A He interstitial and a W SIA were introduced in the system at random in 3 independent runs.

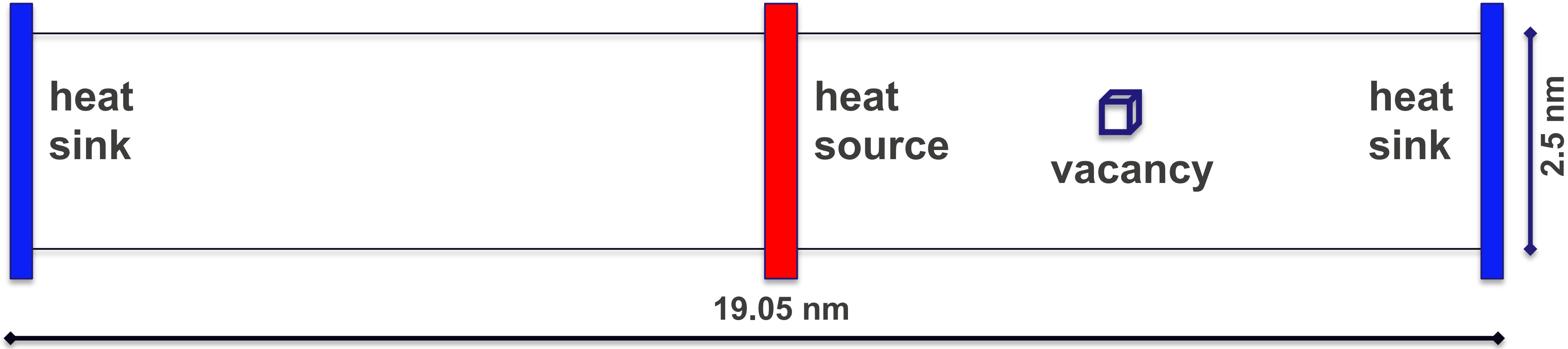
The figure shows a similar exponential decay for the concentration of both He and SIA as obtained with NEMD.

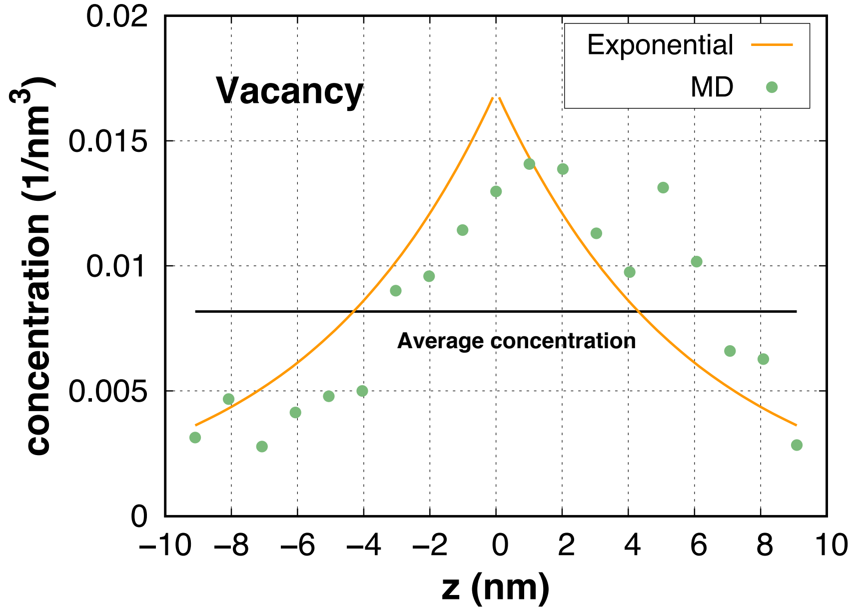
$$c_s = 0.012 \exp(0.17z), \quad \forall z \leq 0$$
$$c_s = 0.012 \exp(-0.17z), \quad \forall z > 0.$$

He/SIA tend to go to the hot region of the sample. Simulations are running to refine the profiles.

Computational Methods

- Non-equilibrium molecular dynamics





Vacancy is harder to converge because its mobility is reduced compared to that of He or SIA.

It tends to stay longer in the hot regions as well but the exponential behavior is harder to identify.

In all three cases studied defects and impurity atoms tend to go to the hot regions. It does not seem like there is a simple correlation to the stress/strain state induced by the defect/impurity.

Irreversible Thermodynamics Analysis

- We have used irreversible thermodynamics to rationalize the NEMD results. The heat and atomic species (He atoms or SIAs) fluxes are coupled through the transport coefficients and thermodynamic driving forces

$$\begin{pmatrix} J_q \\ J_s \end{pmatrix} = \begin{pmatrix} L_{qq} & L_{qs} \\ L_{sq} & L_{ss} \end{pmatrix} \begin{pmatrix} \nabla\left(\frac{1}{T}\right) \\ -\nabla\left(\frac{\mu_s}{T}\right) \end{pmatrix} = \begin{pmatrix} L_{qq} & L_{qs} \\ L_{qs} & L_{ss} \end{pmatrix} \begin{pmatrix} \nabla\left(\frac{1}{T}\right) \\ -\nabla\left(\frac{\mu_s}{T}\right) \end{pmatrix}$$

Using Fourier's law, the heat flux can be written as $J_q = -\kappa\nabla T + L_{qs}\nabla\left(-\frac{\mu_s}{T}\right)$

Setting the activity coefficient equal to 1 (dilute limit), the chemical potential can be written as

$$\mu_s = k_B T \ln\left(x_s\right)$$

Therefore, $J_q = -\kappa\nabla T - k_B L_{qs}\frac{\nabla x_s}{x_s}, \quad J_s = -L_{ss}Q_s^*\frac{\nabla T}{T^2} - k_B L_{ss}\frac{\nabla x_s}{x_s}$

with $L_{qs} = L_{ss}Q_s^*$ $\qquad Q_s^*$ **is the heat of transport**

Mass (Atomic Species) Transport Equation

- **Since there is no flux of particles in or out of the system** $J_s = 0$

$$-k_B \frac{\nabla x_s}{x_s} = Q_s^* \frac{\nabla T}{T^2}$$

$$\nabla \ln x_s = -\frac{Q_s^*}{k_B T^2} \nabla T$$

$$\rightarrow \quad x_s = C_0 \exp\left(-\int \frac{Q_s^*}{k_B T^2} dT\right)$$

which decays exponentially as shown by MD

Fitting MD we obtain For both He and SIA $Q_s^* = -0.0081 k_B T^2$

Relating Fick's law with the mass transport equation

$$\frac{k_B L_{ss}}{x_s} \nabla x_s = D_s c_0 \nabla x_s = D_s \nabla c_s \quad \rightarrow \quad L_{ss} = \frac{D_s c_0 x_s}{k_B} = \frac{D_s c_s}{k_B}$$

And substituting $\frac{\nabla x_s}{x_s}$ into the heat flux equation

$$J_q = -\kappa \nabla T \left(1 - \frac{L_{ss} Q_s^{*2}}{\kappa T^2}\right) = -\kappa \nabla T \left(1 - \frac{D C_0 Q_s^{*2}}{k_B \kappa T^2} x_s\right)$$

$$\frac{D C_0 Q_s^{*2}}{k_B \kappa T^2} x_s \ll 1$$

Hence, the heat transport equation can be decoupled from the mass transport equation in the dilute case.

$\kappa(T)$ seems to have a temperature dependence, but it does not change the physics

Transient Effects

- **With a heat of transport available, we can use the balance equations to predict the material response during transients**

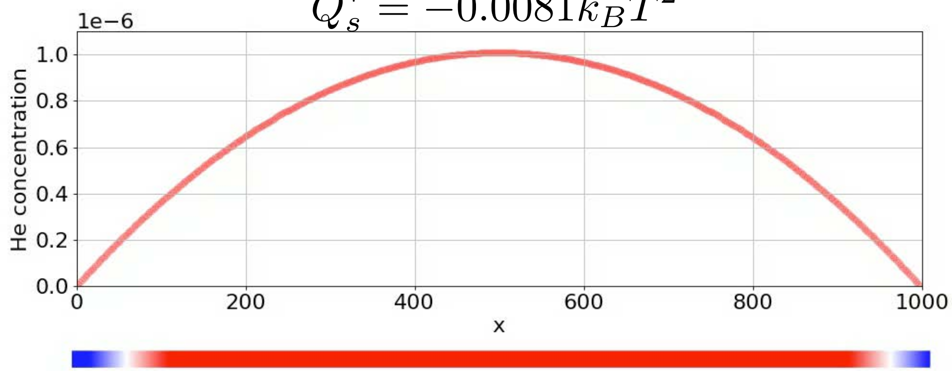
$$\rho c_v \frac{\partial T}{\partial t} = -\nabla \cdot J_q$$
$$\frac{\partial x_s}{\partial t} = -\nabla \cdot J_s + S$$

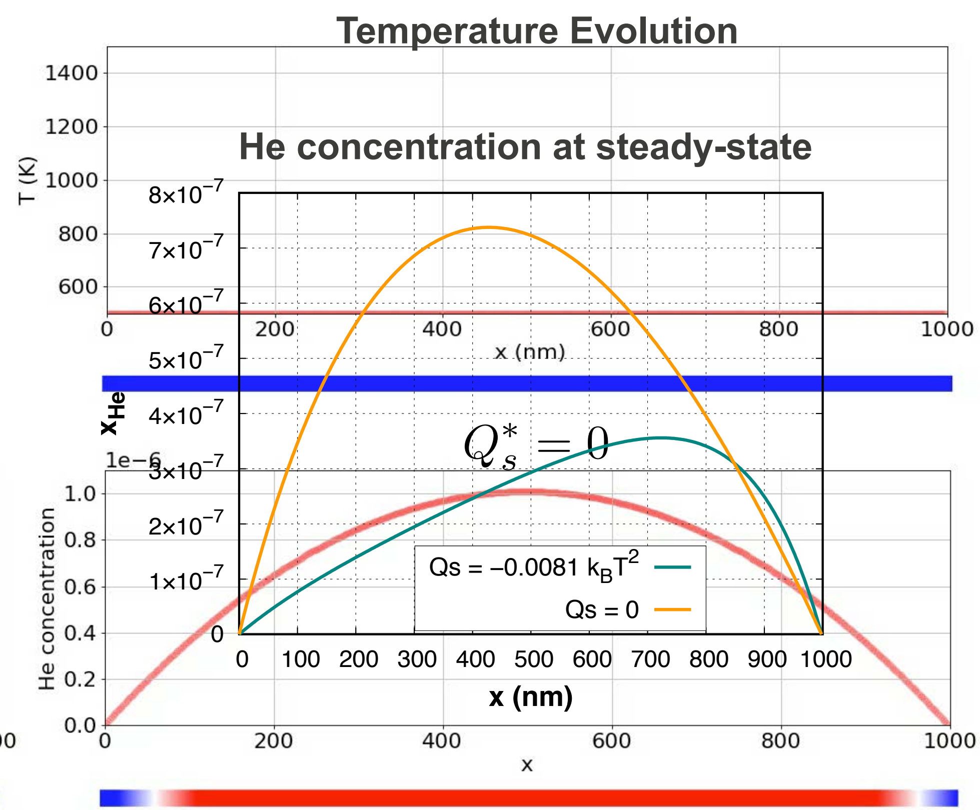
$\rightarrow$

$$\rho c_v \frac{\partial T}{\partial t} = \nabla \cdot \kappa(T)\nabla T$$
$$\frac{\partial x_s}{\partial t} = \nabla \cdot \left(\frac{D_s x_s Q_s^*}{k_B T^2} \nabla T + D_s \nabla x_s \right) + S$$

- κ = Cte.
- Temperature increases in one of the surfaces (boundaries), from the initial 500 to 1500 K (the other one is kept at 500 K).
- The He concentration is set to 0 at the boundaries (ideal sink assumption).
- Homogeneous source of 0.002 dpa/s.
- The size of the beam is 1 μm.

$$Q_s^* = -0.0081 k_B T^2$$





Conclusions

- We have studied the effect of thermal gradients on transport properties of He, V and SIA in W.
- Defects and impurities tend to go to the hot regions of the sample.
- We have been able to compute the heat of transport for each species relying on an nonequilibrium thermodynamics formalism.
- We have analyzed transients and observed a significant effect of the He concentration profile when the flux coupling is used.
- We plan to analyze the coupling for small impurity and defect clusters.

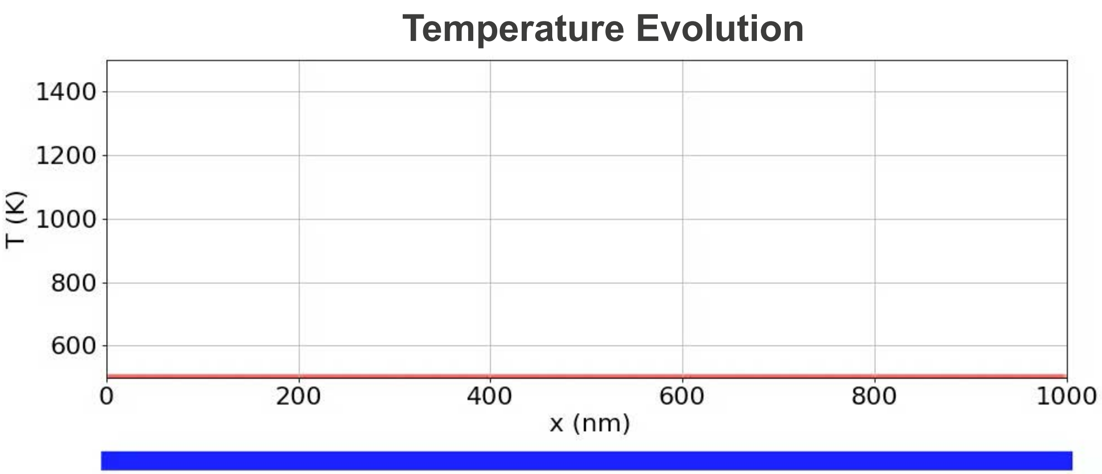
THANK YOU

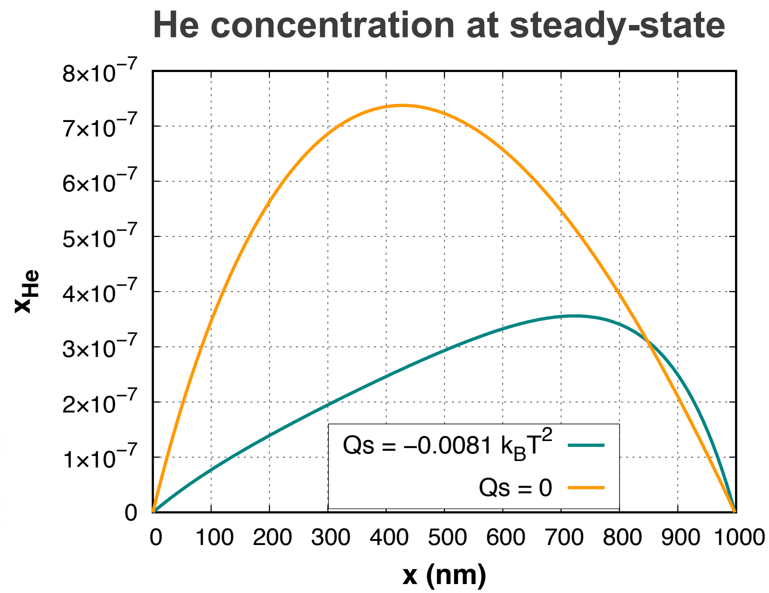
SciDAC
Scientific Discovery through Advanced Computing

Los Alamos
NATIONAL LABORATORY
EST. 1943

Transient Effects

- The final steady-state profiles are shown below, highlighting the impact of the effect (Soret diffusion) in the species distribution in the material





Outstanding questions

- How relevant can this effect be for ELMs and/or disruptions?
- What is the effect of the electronic thermal conductivity (only the lattice thermal conductivity is accounted for in classical MD)?
- What is the origin of the negative heat of transport? Phonon wind?