Nuclear Fusion Reactor Materials: Modelling Atomic-Scale Irradiation Damage in Metal

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EXTENDED ABSTRACT

Achieving nuclear fusion as an energy source on Earth is a practical goal that relies on continuing scientific and engineering innovation. Functional fusion reactors around the world today allow scientists and engineers to plan improvements that will eventually allow for greater energy output than the input required to operate the machine (including heating the plasma and operating the superconducting electromagnets that confine the plasma, among other energy inputs). The fusion reaction between nuclei of hydrogen isotopes is a carbon-free source of massive amounts of energy that could be paramount in a global turn towards greener energy. The fusion fuel needed to provide one person's energy use for 100 years (assuming 20 kWh per day) is contained within roughly one and a half bathtubs of water and 3 laptop batteries. Given the enormous payoff of fusion, continued research and development are of great interest so that current challenges of heating and confining plasma, mitigating plasma disruptions, improving efficiency of magnets, and extending the lifetime of materials subjected to the harsh conditions surrounding the plasma may be overcome. Fusion reactor materials research carried out here at the BSC contributes to this ambitious goal.

The idealistic goal for fusion materials research is to provide predictions about material behavior with the accuracy of quantum mechanical calculations at the scale of a full fusion reactor. Using strategic approximations and working at a small scale, computational fusion materials researchers can accurately reproduce and explain experimentally observed physical phenomena, such as the formation of microstructural defects in metals under neutron-irradiation, and offer the best predictions available for behavior of materials in future fusion reactor environments, where data about what will happen simply do not exist yet.

In the study presented here, we examined the thermal conductivity, or how quickly a material allows heat to flow, of tungsten (W). W has been selected for plasma-facing components in ITER, which is currently under construction. We used LAMMPS atomic modelling of materials software and found that the thermal conductivity of W is significantly decreased in the presence of defects.

A. Introduction

Fusion reactors depend on cutting edge scientific and engineering knowledge. As such, the materials used to build a fusion reactor are carefully designed to fulfill a variety of different purposes [1]. The material that serves as the focal point of this study, tungsten (W), is used in protective plasma-facing components (PFC), which require high melting temperatures and high thermal conductivity among other characteristics. One of the primary purposes of W in the fusion reactor is to carry excess heat away from the plasma quickly without melting and without allowing other nearby components to melt. A PFC called the divertor is expected to undergo extreme heat fluxes of 10-20 MWm^2 during ITER operation. The ability of PFC to dissipate heat is given by their thermal conductivity. Materials like W conduct heat through electrons and phonons (quasiparticles representing vibrations in a crystal lattice). This study considers the phonon thermal conductivity, which is expected to be substantially affected by defects. High energy neutrons (14.1 MeV) are emitted by the plasma due to the nuclear fusion reaction between hydrogen isotopes deuterium and tritium. The neutrons provide energy output by heating special parts of the reactor, but also create damage in the protective materials around the plasma. Typical defects associated with this characteristic fusion-produced neutron-irradiation of W include self-interstitial atoms (SIA, W atoms that crowd the normal empty spaces of the crystalline lattice structure), vacancies (empty points in the lattice where a single W atom is missing), voids, and extended defective microstructures formed by the movement of defects throughout the metal, among others.

Computational methods are needed to make predictions about material behavior in future fusion reactors like ITER where experimental data do not yet exist. Quantum mechanical approaches are highly accurate but computationally expensive, and are typically restricted to ground state calculations of a few hundred atoms. Classical molecular dynamics (MD) is a simplified model of particles moving within an external potential. The interatomic interactions are determined using potentials (fitted to quantum mechanical calculations and sometimes experimental data) to calculate the energy and forces between atoms, which are then used to update momenta and positions. MD codes like LAMMPS [2] allow for simulation of larger systems for longer times at realistic temperatures due to a decreased computational cost. In this study, we used MD to explore how the phonon thermal conductivity of W changes in the presence of defects.

B. Methods

We estimated thermal conductivity of W using LAMMPS and a non-equilibrium molecular dynamics (NEMD) approach based on the classic Fourier heat transfer law:

$$\kappa = \frac{J}{\partial T / \partial x}$$

where κ is the thermal conductivity, J is the heat flux in the x direction, and $\partial T/\partial x$ is the gradient of temperature in the x

direction [3]. We created a simulation cell with 3D periodic boundary conditions containing a few hundred thousand to a few million atoms, corresponding to physical dimensions of 1583 × 158 × 158 Å (one Angström is one tenth of one nanometer) for the largest system. The system was then equilibrated to 300 K and zero pressure using NPT (isothermal-isobaric) and NVT (canonical ensemble) relaxations in LAMMPS. Next, we applied a local heat source and sink to create regions of hot and cold, resulting in a steady state heat flux J after 400 picoseconds of simulated time (400 cpu hours). Between the heat source and sink regions, we placed defects and measured their effect on κ.

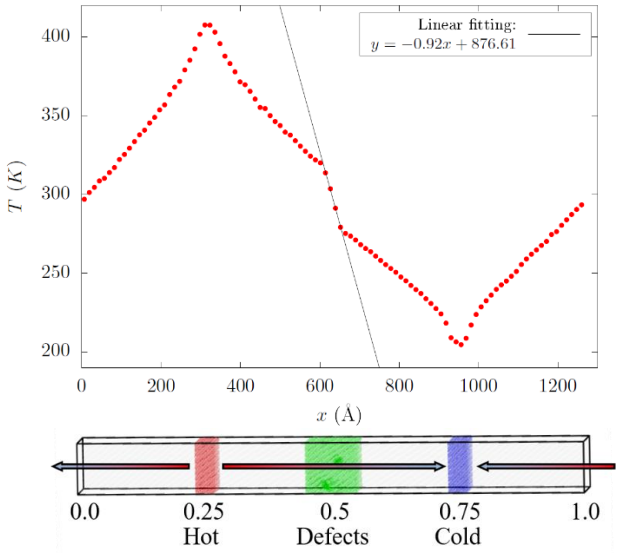

Fig. 1 A sample temperature profile of a W system with a void placed in the center, and a schematic indicating heated and cooled regions and placement of defective material. Arrows indicate the direction of heat flow.

We tested a variety of types of defects including spherical voids in the W lattice and defective microstructures consisting of vacancies and clusters of interstitial atoms. The voids had radii of up to 30 Å, placed in the center of the simulation cell. The effect of a void with radius 20 Å is visible in Fig. 1 as a sharply steeper slope in the temperature profile, signifying a lower thermal conductivity in the damaged region. An initial strategy that we tried for creating the types of defective microstructures associated with high energy neutron-irradiation was a cascade procedure starting with one high energy atom (up to 200 keV). Due to the heavy computational cost of simulating defect cascades, a new simplified method was instead used: Creation Relaxation Algorithm (CRA) [4]. CRA can produce damage levels that are several orders of magnitude higher than defect cascade approaches for similar computational time. This algorithm iteratively inserts Frenkel pairs (one SIA and one vacancy) randomly, then performs an energy minimization by making small adjustments to the positions of all atoms. Building up 250 iterations of inserting 1000 Frenkel pairs then performing the energy minimization required 1200 cpu hours (about 5 cpu hours per minimization) in a 2.5M atom system.

C. Results

For a perfect W system of 320k atoms without structural defects, we found a phonon thermal conductivity of 13.33 W/mK. Thermal conductivity dropped by 74% in the example shown in Fig. 1, where the cross sectional area of the spherical void (circle of radius 20 Å) is about 30% of the cross sectional area of the simulation cell (square of side length 63 Å). A small void where only 11 atoms were removed from a system of half of a million atoms resulted in a 5% decrease in thermal conductivity. In the presence of a highly defective microstructure corresponding to the insertion of one Frenkel pair for every atom within the central damaged region of the simulation cell, W thermal conductivity decreased by 21%.

D. Discussion

One implication of the decreased thermal conductivity of W in the presence of defects is the risk of melting of reactor components due to a build-up of heat on the plasma-facing side. This predicted effect in fusion reactor materials is one way that the lifetime of machine components is limited, reducing the overall efficiency of energy output to machine maintenance in future fusion power plants.

This work can be extended by using alternative methods for estimating thermal conductivity, such as the Green-Kubo equilibrium molecular dynamics approach. A wider range of temperatures could be examined, since operating conditions of W in ITER will include 1200-1600 K. Further, voids could be filled with gases expected inside fusion reactors, such as the helium that results from the nuclear fusion of deuterium and tritium. Another major avenue to extend this work will be to compare results given alternative interatomic potentials.

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Author biography

Mary Kate Chessey completed a BSc in physics at Drexel University (Philadelphia, USA) in 2013, and a MSc in physics and PhD in physics education research in 2018 at the University of California Davis. She was then a Postdoctoral Research Associate at University of Maryland College Park. In 2021 she joined the CASE Department at the BSC, working most closely with Dr. Julio Gutiérrez in the Fusion Group led by ICREA Prof. Mervi Mantsinen.