Improving Long Term Stability of Nuclear Power

An investigation into defect resistant materials for use in nuclear reactors and other high radiation environments.

Nuclear energy has long been regarded as a practically unlimited source of energy. For years, the developed world has been largely powered by nuclear energy, an exceptionally clean and sustainable fuel source. Nuclear fuel is affordable and abundant, possessing an incredibly high energy density–over one million times that of gas and diesel [2]. The longterm sustainability of nuclear power is not an issue of abundance, but one of materials science.

As nuclear reactors age, the structural integrity of reactor bodies degrades as a result of the high energy neutrons, an unavoidable side effect of the nuclear chain reaction. The containment unit of a nuclear reactor is continuously subjected to extremely high energy neutron radiation. This radiation can cause abundant defects [4] such as atomic vacancies (missing atoms), and bubbles of accumulated hydrogen and helium. These defects weaken the structural integrity of the reactor, reducing its reliability and its lifetime. A clear understanding of materials with such defects is essential to the long-term economic sustainability of nuclear power.

Recently, advances in such understanding have been made by researchers at Universidad de Oviedo, Spain and Massachusetts Institute of Technology (MIT), in the United States [3]. They investigated the interfacial areas between copper and niobium, prospective materials for future reactor design. It is known that metallic structures abundant in interfaces – locations where two different materials are in contact – are highly resistant to defects [1]. Atoms in the crystalline copper and niobium have very well-defined crystal structures. Copper is face-centered-cubic (FCC) and niobium is body-centered-cubic (BCC). When neutrons collide with the crystal atoms, they can knock atoms out of their well-defined positions, creating defects in the crystal. Dr. M. Demkowicz at MIT explains that there are two types of defects: vacancies, and interstitials. A vacancy is the absence of an atom in a position where, structurally, there is expected to be one. An interstitial is an additional atom present in the crystal structure, in between the normal structure. He explains that these defects can accumulate, growing larger and degrading the quality of the material. This damage is not, however irreparable. If an interstitial atom migrates close enough to a vacancy, the interstitial can "fill in" the position of the vacancy, effectively repairing the defect, Dr. Demkowicz says. The problem is that, in a three dimensional crystal, the rate at which interstitials and defects combine is much lower than the rate of defect creation, leading to a surplus of defects.

If a defect manages to make it to an interfacial region, it is confined there by a potential energy barrier. Interfacial regions in materials provide a location for both types of defects to accumulate and subsequently annihilate. Dr. Demkowicz explains that since the interface restricts the defects to two dimensional motion, the recombination rate is much greater than in the bulk material. He compares the process to the way a catalytic converter in a car traps oxygen, and toxic carbon monoxide, combining them to form inert carbon dioxide. The interface acts as a catalyst, trapping defects and allowing them to recombine at much higher rates than in the bulk material.

By using a density functional theory-based approach, he and his team analyzed the stability and energetic properties of point defects in such materials.

Density functional theory (DFT) is an approximate computational method used to solve the complicated Schrödinger equation of quantum mechanics, an equation too difficult to solve exactly for large systems of atoms. Even with the approximations and simplifications of DFT, it can only be used to simulate a few hundred atoms at a time, making it difficult to model macroscopic properties like interfaces and boundaries between different metals in the material. They decided to model a copper-niobium interface made up of 324 Cu atoms and 240 Nb atoms, arranged in a total of 12 layers (Figure 1). They investigated both vacancies and interstitials using the nudged elastic band (NEB method). According to Dr. Demkowicz, the NEB method gives a reliable indication of the energy required for a defect to follow a specific migratory route toward the interface. He explains, “as the [defect] moves around, it passes through a state of elevated energy”, eventually coming to rest at the interface between materials. Calculating this energy allowed them to find the most preferred diffusion pathway.

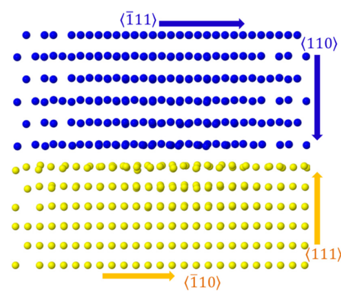

Figure 1: The 12-layer system of Cu (yellow) and Nb (blue) atoms.

They ran 90 simulations, with defects placed at various locations and tracked the path and energy requirements of defect migration. They found that defects do indeed progress toward the interfacial boundary; the interface corresponds to a lower potential energy. Once there, they confirmed that the defects become trapped at the two-dimensional surface because of the high potential energy barrier. They remain there until a complementary defect migrates within close proximity, facilitating annihilation.

Dr. Demkowicz views the results as a successful characterization of the Cu/Nb interface. Their results agreed well with experimental observations. He also indicated that it gave them insight into the specific migratory routes that defects take toward the interface, possibly allowing future materials to be tuned to allow efficient transport.

Dr. Demkowicz and his team are continuing to investigate other similar materials, specifically the interfaces of other face-centered and body-centered cubic structures in an effort to observe similar properties in other materials. Their work could help improve the stability and longevity of nuclear reactors, providing clean, safe energy for years to come.

–Kyle Mills

References

[1] Demkowicz, M. J., Hoagland, R. G., and Hirth, J. P. *Phys. Rev. Lett.*, 100(April):2–5, 2008.

[2] Eerkens, J. W. *The Nuclear Imperative*. 2010.

[3] González, C., Iglesias, R., and Demkowicz, M. J. *Phys. Rev. B*, 91:1–7, 2015.

[4] Zinkle, S. J. and Busby, J. T. *Mater. Today*, 12(11):12–19, 2009.