# Supplementary Material:
# Effects of Galactic Irradiation on Thermal and Electronic Transport in Tungsten

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**Abstract**

The impact of irradiation on the thermal and electronic properties of materials is a persistent puzzle, particularly defect formation due to primary knock-on atoms (PKAs). This work examines the nanoscale effects of low-energy irradiation on tungsten (W), focusing on defect-induced modifications to thermal and electronic transport. Using the Space-Projected Thermal Conductivity (SPTC) method [A. Gautam *et al.* PSS-RRL, 2400306, 2024], we analyze bulk and twin-grain boundary W with vacancy defects based on the Norgett-Robinson-Torrens displacements per atom (NRT-dpa) model. SPTC provides a detailed prediction of post-cascade spatial thermal conductivity distribution. We estimate electronic conductivity activity using the "$N^2$ method" [K. Nepal *et al.* Carbon, 119711, 2025] to explore the consequences of vacancies and grain boundaries, highlighting the defect-dependent nature of charge transport behavior. These findings offer high-resolution insights into irradiation-driven transport phenomena, with implications for space-exposed materials and nanoscale thermal/electronic management.

## Sect. S1. Description of the Supporting Figures

The figures provided herein supplement the discussion in the main text. The site-projected thermal conductivity (SPTC) distributions for the twin grain boundary models—TGB, TGB1SV, and TGBDV—are shown in Figure S1a, b, and c, respectively. The left panel serves as a guide for distinguishing atoms in the mirror plane (brown spheres) from the rest (blue spheres). In the model with a single vacancy, TGB1SV (Figure S1b), the vacancy site is identified by a gray sphere. In TGBDV, the vacancy sites are marked by black and gray spheres. The SPTC distribution is shown in the right column, with the colorbar indicating SPTC values normalized to the bulk maximum and expressed as a percentage. Thus, it can be interpreted as the "recovery rate" of thermal activity from the defect-affected region to bulk-like behavior.

The electronic conduction distributions in specific planes of the twin grain boundary models, obtained from $N^2$ calculations, are shown in Figure S2 for TGB, TGB1SV, TGB2SV, and TGBDV in rows I, II, III, and IV, respectively. The $N^2$ projections are represented for five atomic planes located at $z \approx$ (a) 2.24, (b) 4.48, (c) 6.71, (d) 8.95, and (e) 11.19 Å. Atomic sites are represented by blue circles, while white arrows mark vacancy locations. Similarly, the electronic conduction distributions for the bulk models are shown in Figure S3, corresponding to the Bulk, Bulk1SV, Bulk2SV, and BulkDV models in rows I, II, III, and IV, respectively. Only atomic planes matching the columns in Figure S2 are considered.

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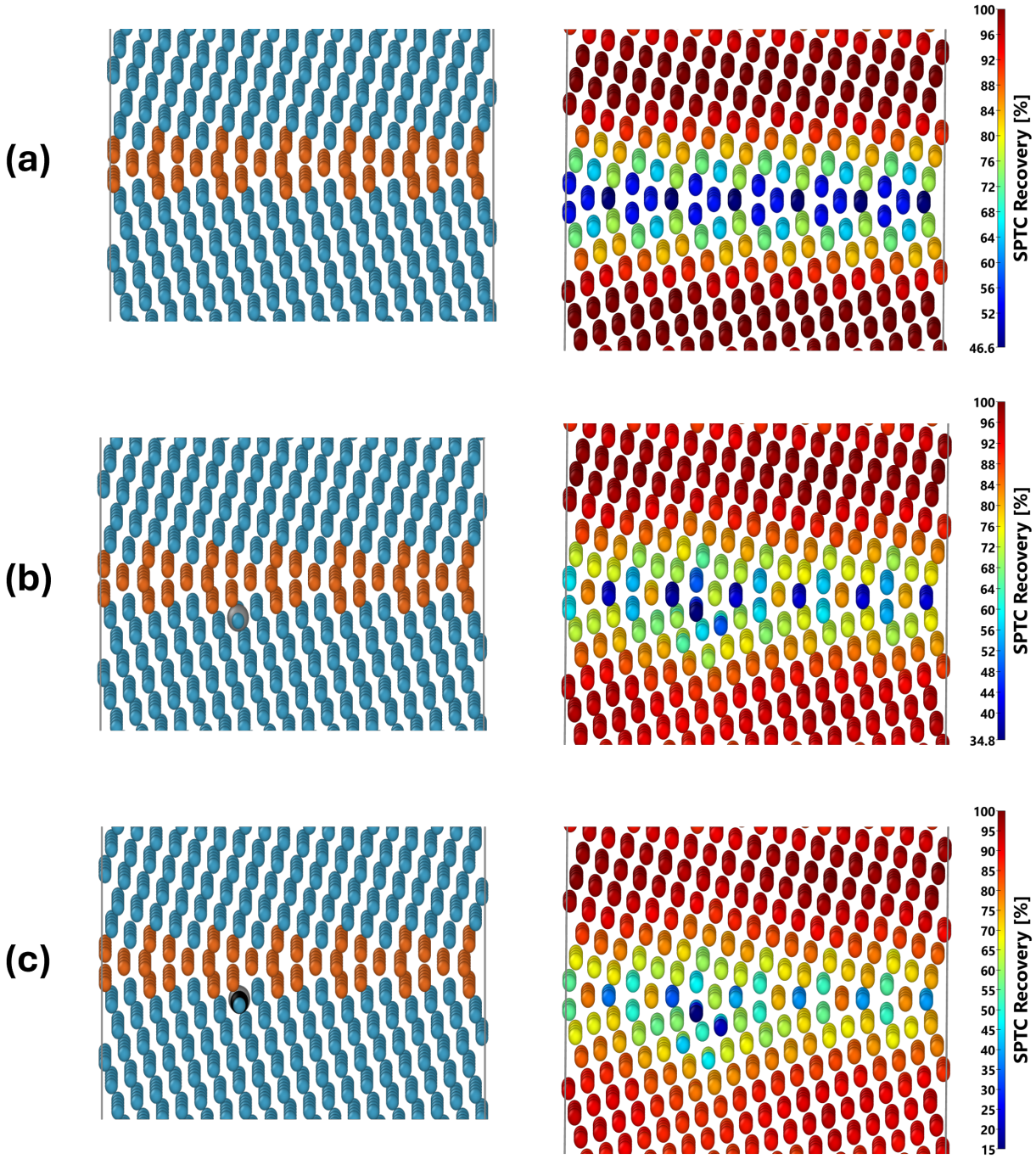


Figure S1: Thermally active sites in W twin grain boundary models: (a) TGB, (b) TGB1SV, and (c) TGBDV. The left column, which guides the SPTC trend in the right column, shows the atoms in the mirror plane in brown and the rest in blue. the vacancy sites are colored gray (and black in (c)). The colorbar shows the SPTC recovery to its maximum away from the mirror plane or defect.

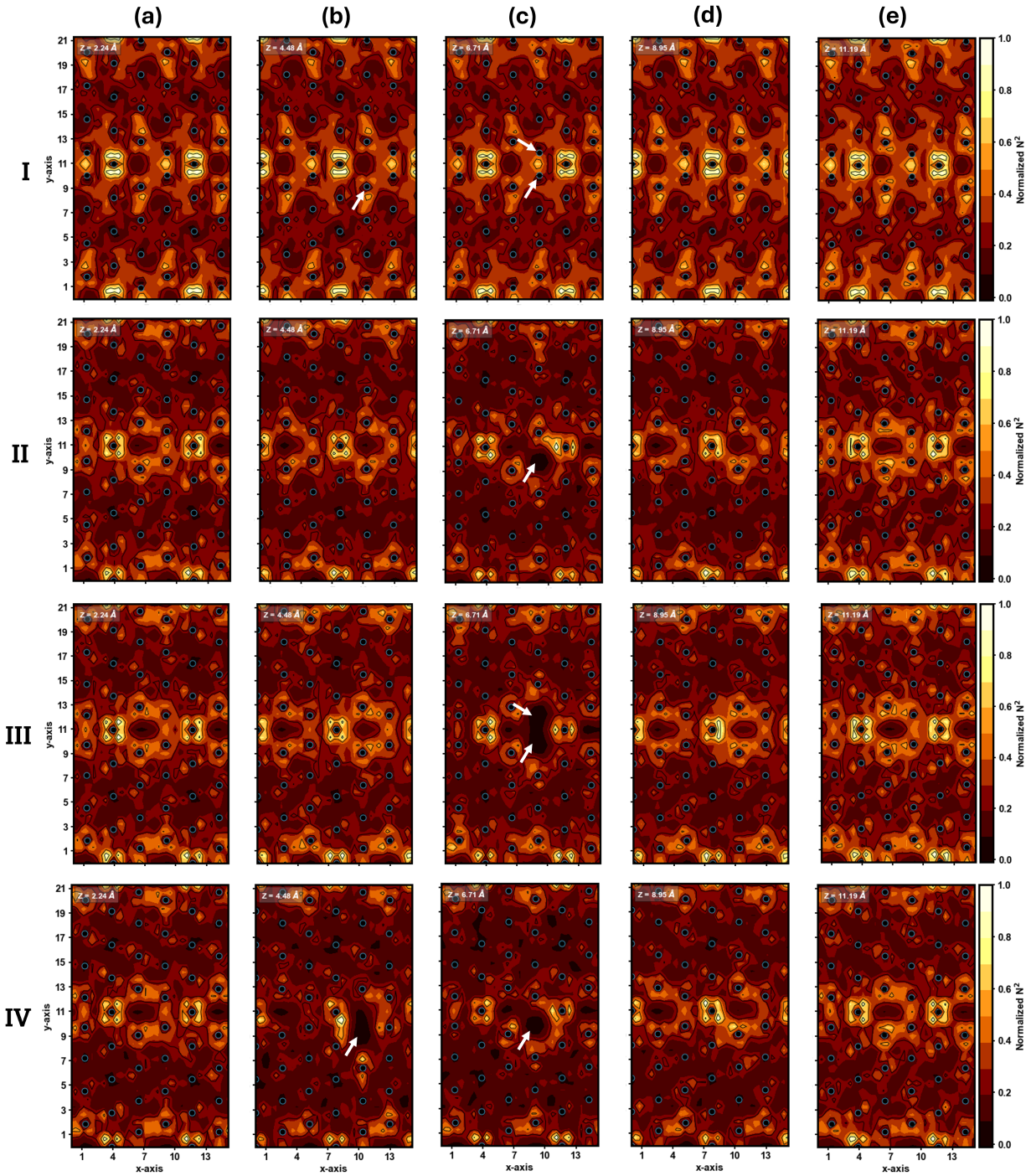


Figure S2: Normalized $N^2$ values for electronic conduction paths in W twin grain boundary models: [I] TGB, [II] TGB-1SV, [III] TGB-2SV, and [IV] TGB-DV. White arrows indicate vacancy sites and blue circles represent atom positions.

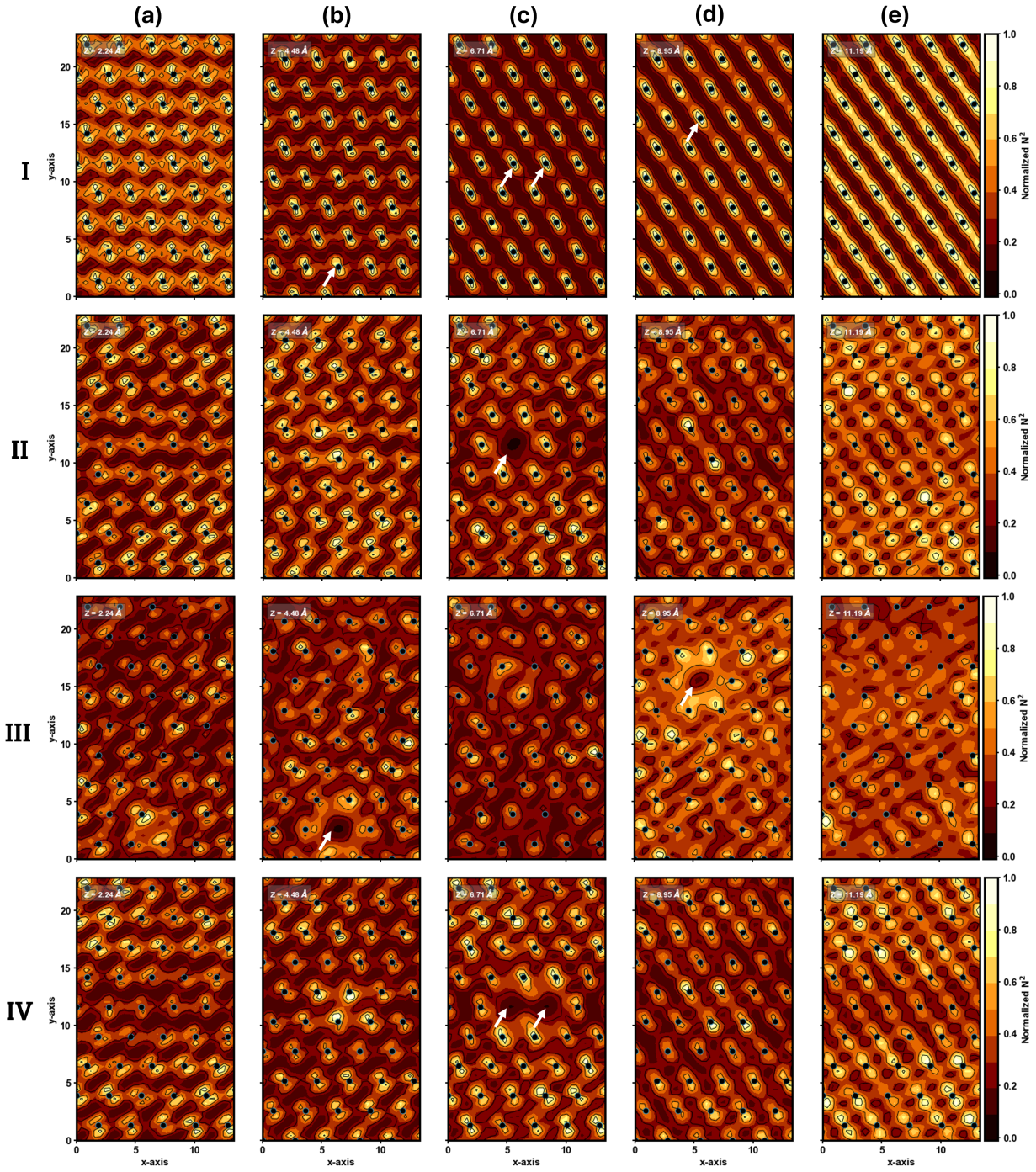


Figure S3: Normalized $N^2$ values for electronic conduction paths in the bulk W models: [I] Bulk, [II] Bulk-1SV, [III] Bulk-2SV, and [IV] TGB-DV. White arrows indicate vacancy sites. Blue circles represent atom positions.