

# Computational Analysis of Composite Thermoelectric Materials for Energy Conversion Applications

R. G. Cherkez, O. M. Porybanyi

Yuriy Fedkovych Chernivtsi National University, Chernivtsi, Ukraine

r.cherkez@chnu.edu.ua

§ 7  
Section

## Introduction

One of the promising approaches for improving the performance of thermoelectric materials is the development of **composite structures** that combine a thermoelectric matrix with secondary phases possessing different transport properties. The presence of such inclusions can significantly affect charge carrier transport and therefore modify the effective electrical and thermoelectric characteristics of the material [1–3]. Thermoelectric composites attract growing interest due to their potential for independent tuning of electrical and thermal transport, enabling higher figures of merit  $ZT$  compared to single-phase materials.

## Methodology

A **finite-element numerical investigation** of the effective electrical conductivity of a thermoelectric composite was performed using the **Representative Volume Element (RVE) approach**. The RVE is a statistically representative sub-volume of the heterogeneous material that captures the essential microstructural features without modelling the entire macroscopic domain.

Simulations were carried out in **COMSOL Multiphysics 6.1** using the Electric Currents physics interface, which solves the steady-state charge transport equation:

$$\nabla \cdot (\sigma \nabla V) = 0$$

where  $\sigma$  is the local electrical conductivity and  $V$  is the electric potential. Periodic boundary conditions were imposed on opposite faces of the RVE to enforce macroscopic uniformity, while a unit potential difference was applied along the measurement direction to extract the effective conductivity via volume averaging of the resulting current density. The composite microstructure was generated by randomly placing **spherical insulating inclusions** within a conductive thermoelectric matrix ( $\text{Bi}_2\text{Te}_3$ -based alloy,  $\sigma = 1.0 \times 10^5 \text{ S/m}$ ), with inclusion conductivity set three orders of magnitude lower. The mesh was refined near inclusion surfaces to accurately capture the steep potential gradients. A mesh independence study confirmed that results varied by less than 0.5% upon further refinement.

## Key Microstructural Parameters

Parameter	Role	Influence
Inclusion size	Scattering path	High
Volume fraction	Blockage ratio	High
Spatial distribution	Percolation	Moderate
Matrix conductivity	Baseline	High
Inclusion shape	Field distortion	Moderate

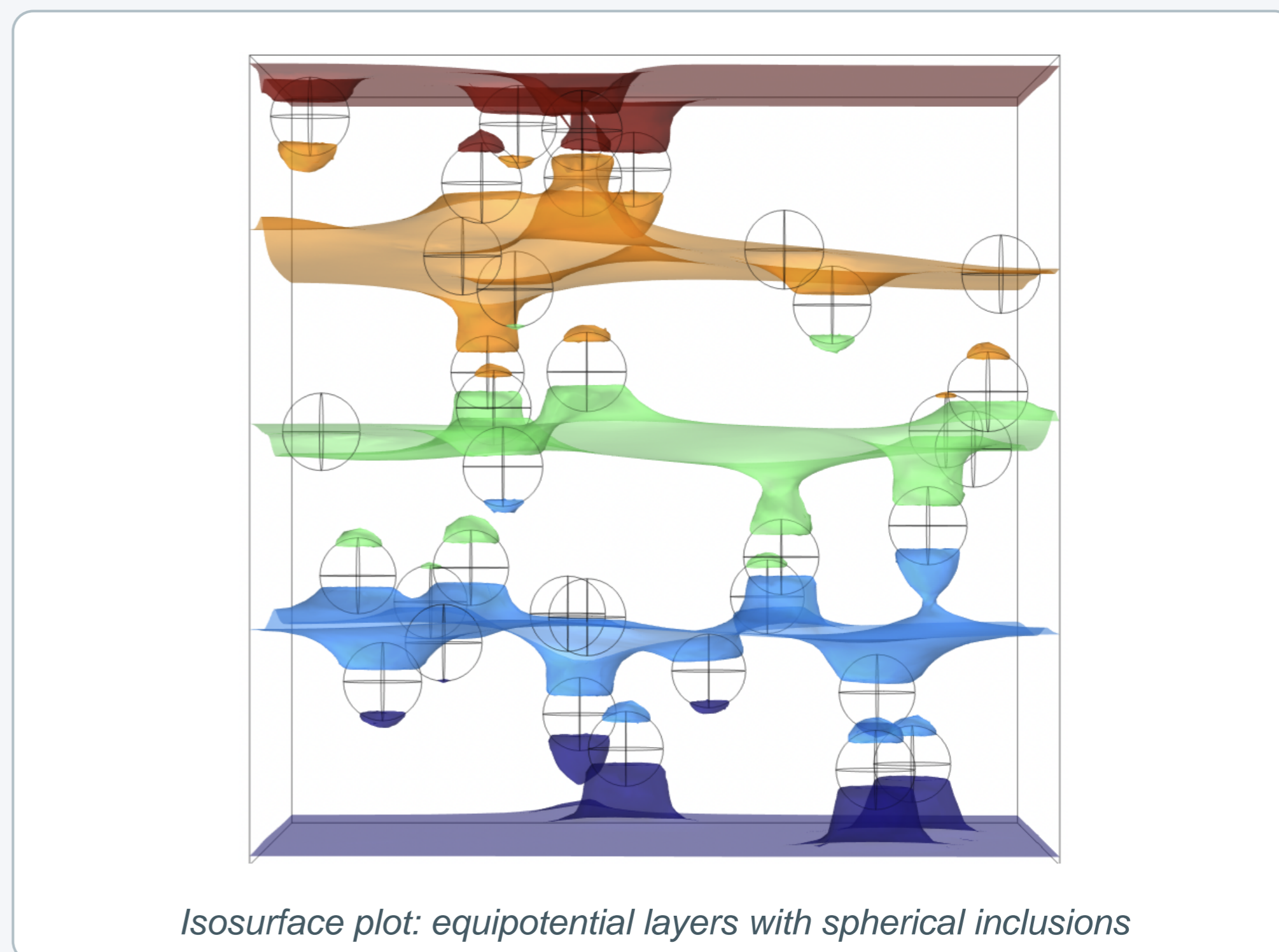
## Results & Discussion

The numerical results reveal that **insulating inclusions profoundly modify the local electric field distribution** within the composite. Electric current is forced to circumvent low-conductivity regions, leading to the formation of complex, tortuous conduction pathways inside the matrix phase. As a consequence, the **effective electrical conductivity of the composite decreases systematically** with increasing inclusion volume fraction, consistent with classical effective-medium predictions.

The isosurface plot (Fig. 1) clearly visualises the stratification of equipotential layers. Near each spherical inclusion the equipotentials are locally compressed, indicating intensified current density in the narrow matrix channels between adjacent inclusions. At higher volume fractions these channels merge and begin to form a connected low-resistance percolation network, which partially counteracts the blocking effect and introduces a nonlinear dependence of  $\sigma_{\text{eff}}$  on inclusion content.

Parametric studies show that for a fixed volume fraction of 20 vol.%, reducing the mean inclusion diameter from 50  $\mu\text{m}$  to 10  $\mu\text{m}$  increases the number density of scattering interfaces and lowers  $\sigma_{\text{eff}}$  by an additional 8–12%, demonstrating the **size-dependent nature** of the blocking effect.

Fig. 1 — Electric Potential Distribution in the RVE (COMSOL)



## Conclusions

The developed **finite-element RVE model** successfully reproduces the reduction of effective electrical conductivity in thermoelectric composites due to insulating inclusions. It demonstrates that microstructural parameters — **inclusion size, volume fraction, and spatial distribution** — play a decisive role in determining effective transport properties. The presented modelling approach offers a systematic tool for predicting and optimising the electrical performance of heterogeneous thermoelectric materials, contributing to the rational design of next-generation energy-conversion composites.

## References

- [1] Z. L. Wang et al., "Knowledge extraction and performance improvement of  $\text{Bi}_2\text{Te}_3$ -based thermoelectric materials," *Nano Energy*, vol. 109, 2023. [2] M. A. Okirigiti, "Recent advances in thermoelectric materials and devices," *Journal of Powder Materials*, 2024. [3] L. Ferretti et al., "Sustainable thermoelectric