A Modelling Framework for Understanding Screen-Printing of Copper Pastes in Solar Cell Metallisation

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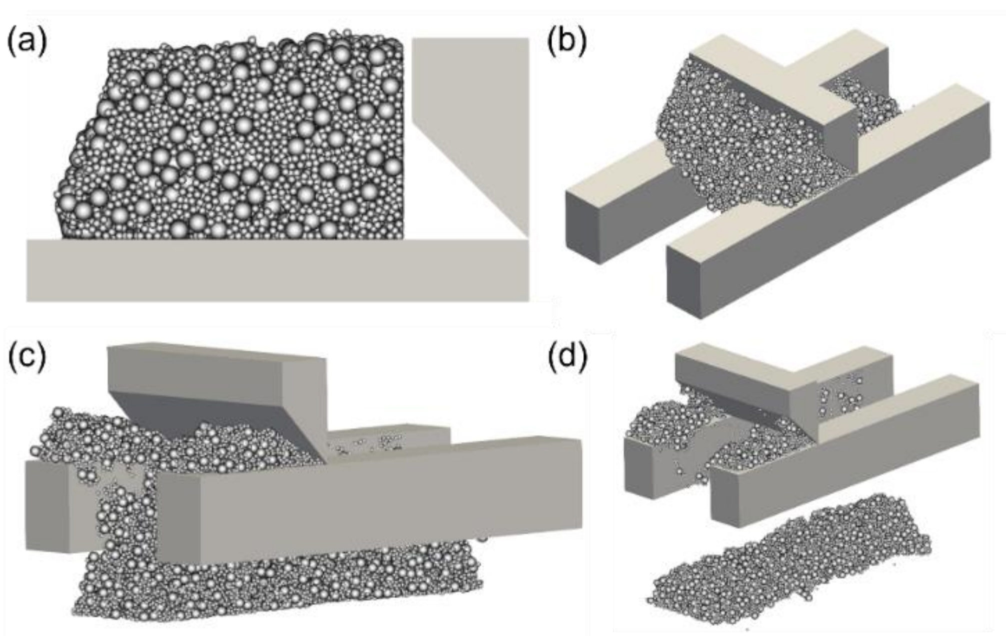
Introduction

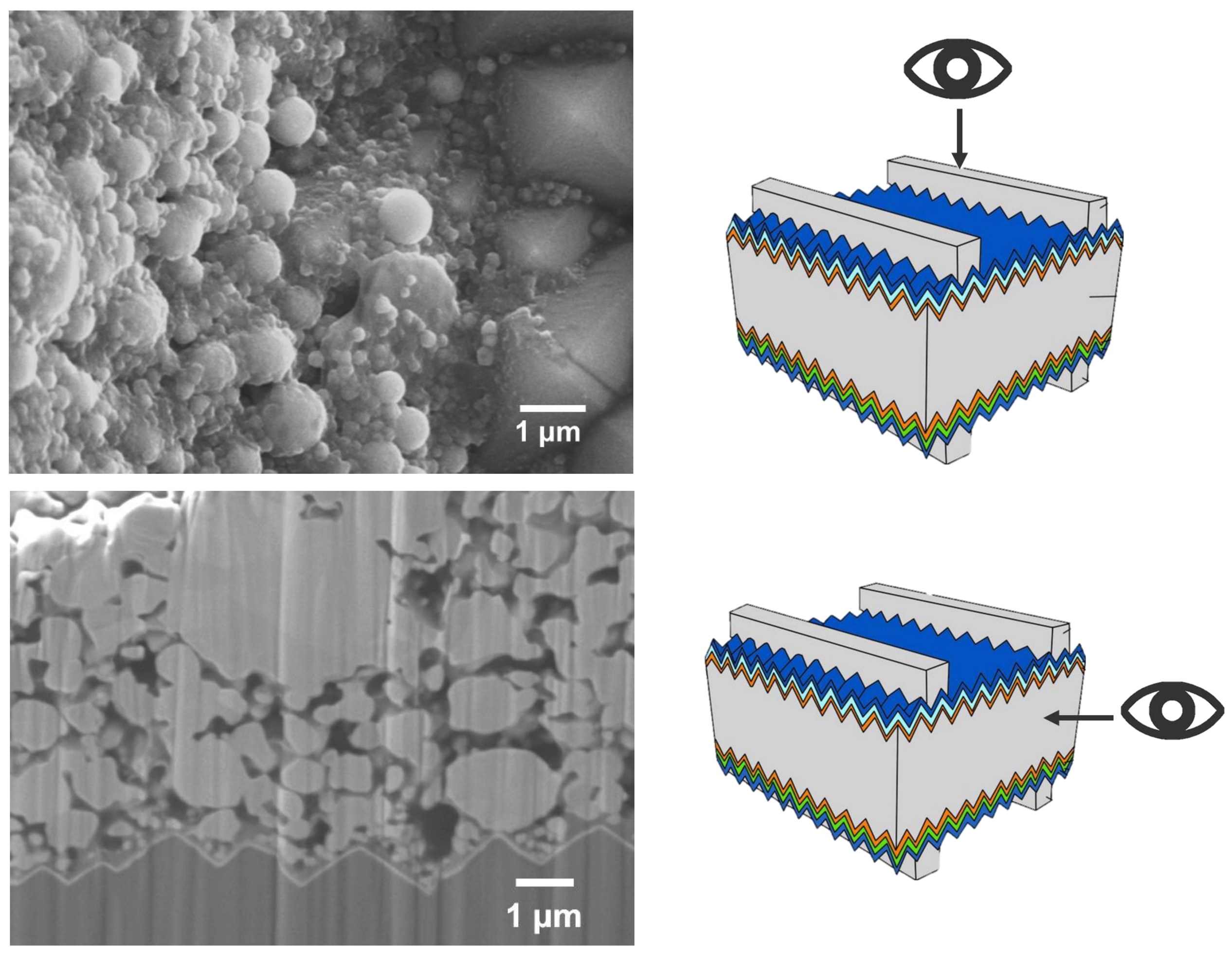
- Copper is a promising replacement for unsustainable silver metallisation.
- Screen-printed copper pastes suffer from limited conductivity.
- Therefore, we developed a modelling approach to predict and improve the conductivity of screen-printed copper pastes.

Methods

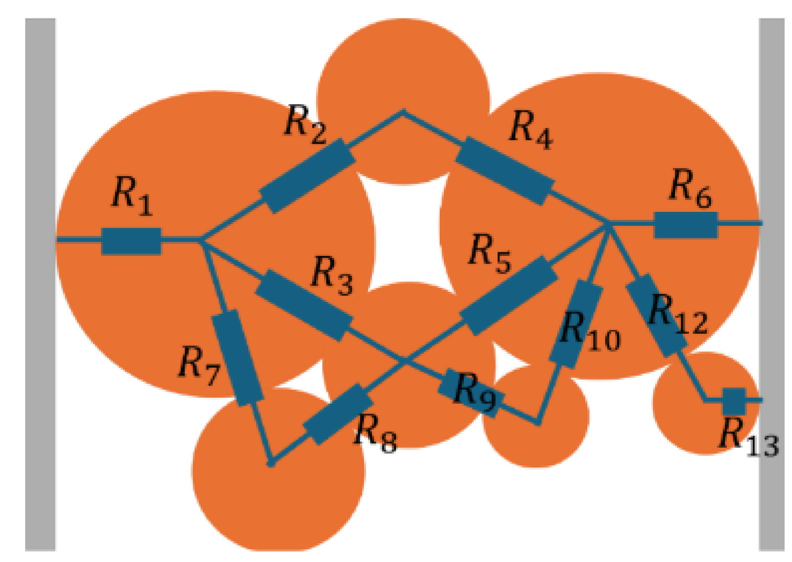
- **DEM simulation of Cu screen-printing** (deposition → squeegee → lift-off → relaxation) using LIGGGHTS.
  - Particle interactions modelled with cohesive forces calibrated to Cu paste morphology.



- **SEM imaging**
- SEM used to gain insight into experimental morphology.

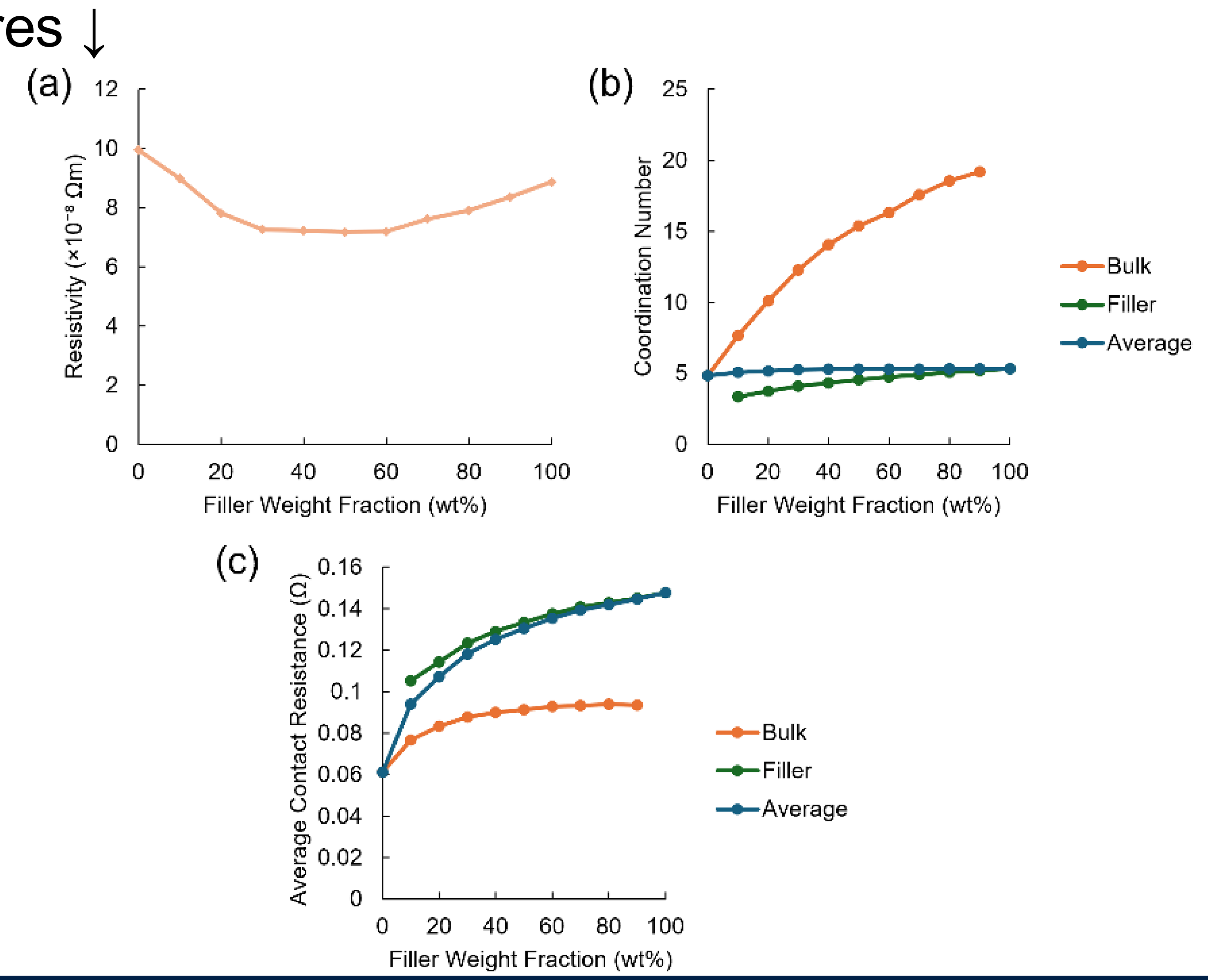


- **Resistive network model** built from geometric solution [1]; resistivity calculated via NetworkX (Kirchhoff's laws).



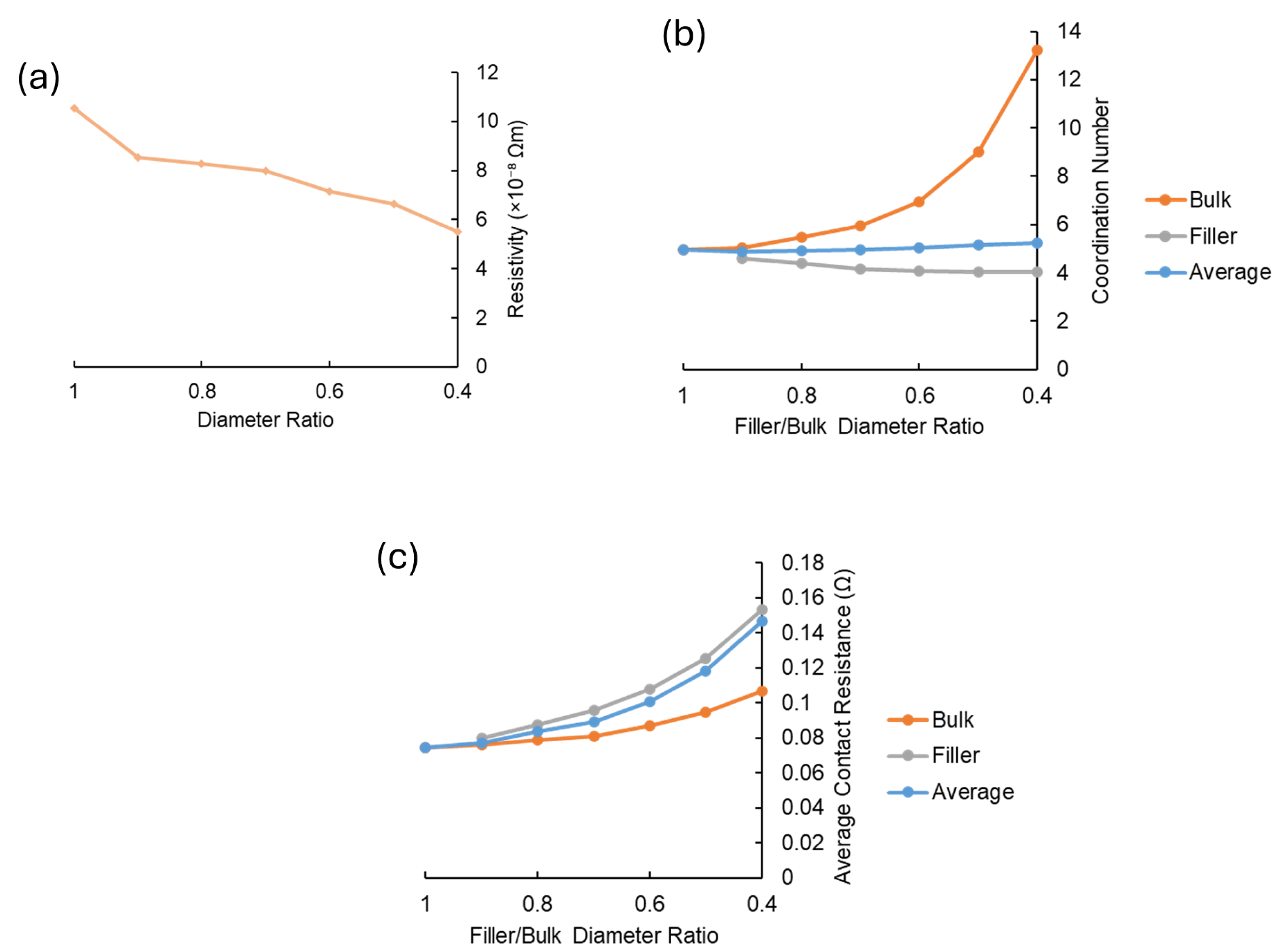
The Effect of Particle Distribution

- Bimodal Cu mixtures with varied filler size and fraction.
- Smaller fillers bridge bulk particles, consistent with SEM.
- Bulk particles provide conductive hubs; fillers improve connectivity.
- Minimum resistivity at **40–60 wt% filler**, matches experimental findings [2].
- Filler addition → coordinated bulk particles ↑ → enables parallel current pathways.
- Excess filler → contact resistance ↑ → bulk conductive centres ↓



The Effect of Particle Sizes

- Filler diameter varied: 0.4–1 µm (bulk = 1 µm, 30 wt% filler).
- Resistivity ↓ with decreasing diameter ratio.
- Coordination number (N_c) roughly constant overall, but doubles for bulk particles as d_r ↓
- Smaller fillers → packing density ↑ → connectivity ↑ → resistivity↓



Conclusions

- DEM + resistive network model successfully predicts Cu paste resistivity.
- Higher coordination → more parallel paths → lower resistance.
- Enables fast, low-cost optimisation of sustainable Cu metallisation.

[1] Rojek et al., *Powder Technol.*, 405, 117521 (2022). [2] Tang et al., *J. Nanoparticle Res.*, 23(8), 166 (2021).

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