

Machine Learning Potentials for Fe-Ni Alloys: Physics-Informed Training via Special Quasirandom Structures

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Background: Machine learning interatomic potentials (MLIPs) enable scalable molecular dynamics simulations, yet achieving accuracy, transferability, and computational efficiency simultaneously remains challenging. Foundation models offer broad chemical coverage but often fail on critical phenomena like structural phase transitions.

Aims: Develop a methodology that combines data-driven neural networks (MACE) with physics-informed chemical sampling to produce interatomic potentials competitive with expensive foundation models while remaining tractable on HPC systems.

Method: We trained equivariant neural networks (MACE) on Special Quasirandom Structures (SQS) for the Fe-Ni system. SQS configurations efficiently tile compositional space, enabling targeted fine-tuning of pre-trained foundation models (OMat-PBE base). Validation encompassed equation of state, elastic constants, bcc to hcp phase transitions at high pressure, and finite-temperature molecular dynamics.

Results: MACE-SQS achieved 30–50% lower errors on elastic constants compared to all tested foundation models (mpa0, OMat, MatPES-PBE, MatPES-r2SCAN). Finite-temperature MD predictions aligned with ab initio molecular dynamics reference data, validating transferability to unseen conditions. SQS training minimized data redundancy compared to random sampling, enabling rapid convergence on HPC clusters.

Conclusion: Physics-informed chemical configuration selection bridges data-driven and physics-based modeling. Strategic SQS sampling yields MLIPs competitive with expensive foundation models while remaining computationally efficient on massively parallel systems. This approach advances predictive modeling for materials discovery and extreme-condition applications in geophysics and materials engineering.