# Article information:

Phys. Rev. B 90, 184301 (2014) - Calculation of strain effects on vacancy-mediated diffusion of impurities in fcc structures: General approach and application to ${\mathrm{Ni}}\_{1\ensuremath{-}x}{\mathrm{Si}}\_{x}$
<https://journals.aps.org/prb/abstract/10.1103/PhysRevB.90.184301>

# Article summary:

1. This article presents an analytical method to calculate the strain-dependent Onsager matrix, which describes vacancy-mediated diffusion of impurities in face-centered cubic structures under elementary strains.

2. The authors show that the atomic scale symmetry breaking induced by strain changes diffusion behavior qualitatively, and that the terms of the Onsager matrix are found to be non-Arrhenian.

3. Nonlinear effects leading to a solute drag reduction are identified for the Ni(Si) alloy under tetragonal strain.

# Article rating:

May be slightly imbalanced: The article presents the information in a generally reliable way, but there are minor points of consideration that could be explored further or claims that are not fully backed by appropriate evidence. Some perspectives may also be omitted, and you are encouraged to use the research topics section to explore the topic further.

# Article analysis:

This article is a well-researched and comprehensive study on the calculation of strain effects on vacancy-mediated diffusion of impurities in fcc structures. The authors present an analytical method—the self-consistent mean field method—to compute analytical expressions of the Onsager matrix describing vacancy-mediated diffusion of impurities in face-centered cubic structures under elementary strains. They also provide evidence for their claims, such as showing that the atomic scale symmetry breaking induced by strain changes diffusion behavior qualitatively, and that nonlinear effects leading to a solute drag reduction are identified for the Ni(Si) alloy under tetragonal strain.

The article is reliable and trustworthy overall, as it provides evidence for its claims and presents both sides equally. However, there are some potential biases that should be noted. For example, while the authors discuss how their results can be used to compute transport coefficients required for accurate mesoscopic simulations of kinetics or to predict macroscopic diffusion kinetic behavior, they do not explore any counterarguments or possible risks associated with this approach. Additionally, while they discuss how their results can be used to investigate strain sensitivity of transport, they do not provide any evidence or examples to support this claim.

In conclusion, this article is generally reliable and trustworthy; however, there are some potential biases that should be noted when considering its content.

# Topics for further research:

* Mesoscopic simulations of kinetics
* Macroscopic diffusion kinetic behavior
* Solute drag reduction
* Strain sensitivity of transport
* Atomic scale symmetry breaking
* Onsager matrix calculations

# Report location:

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