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Crystal Structures and Thermoelectric Properties of Al-Doped β-$FeSi_2$

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INTRODUCTION & AIM

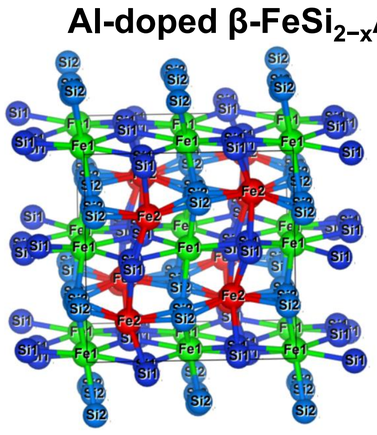
β-$FeSi_2$
- Semiconductors
- Abundant
- Eco-friendly
- Thermoelectrics

Doping (Al)
- p-type control
- Carrier tuning
- Power factor ↑

Challenges
- Secondary phases
- β-phase stability
- Dopant solid solutions [1]

This study's aim
- Crystal structures evolution
- Phase observation
- Thermoelectric properties

Al-doped β-$FeSi_{2-x}Al_x$



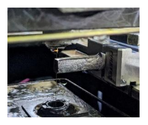
METHOD

Sample preparation

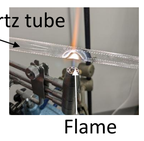
Weighing raw materials (Fe, Si, Al)

Arc-melting (20g)

NC wire cut (7.0 mm × 1.5mm, 7.0 mm)



Vacuum sealing in quartz tube



Heat treatment 1423 K, 3 h, and 1113 K, 20 h

Furnace 1423 K, 3 h, and 1113 K, 20 h

Measurement

XRD by Smart Lab, Rigaku
Rietveld analysis by RIETEN-FP

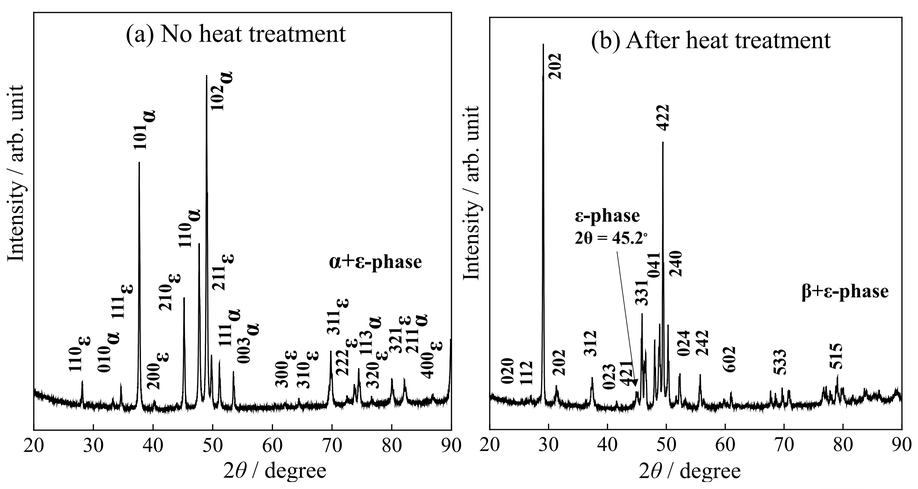
3D SEM VE-8800

Resistivity and Seebeck coefficient by ResiTest 8300 and homemade apparatus

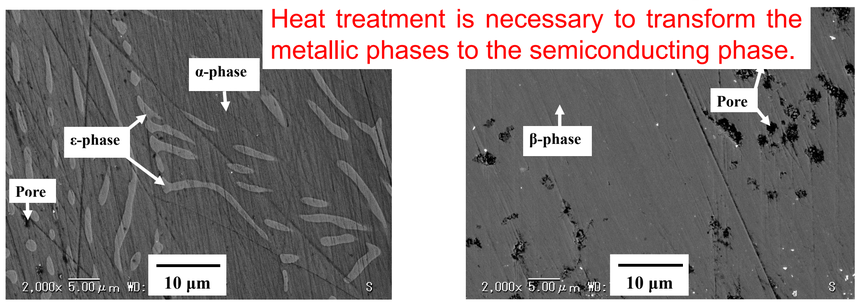
Thermal conductivity by power efficiency measurement (PEM-2)

RESULTS & DISCUSSION

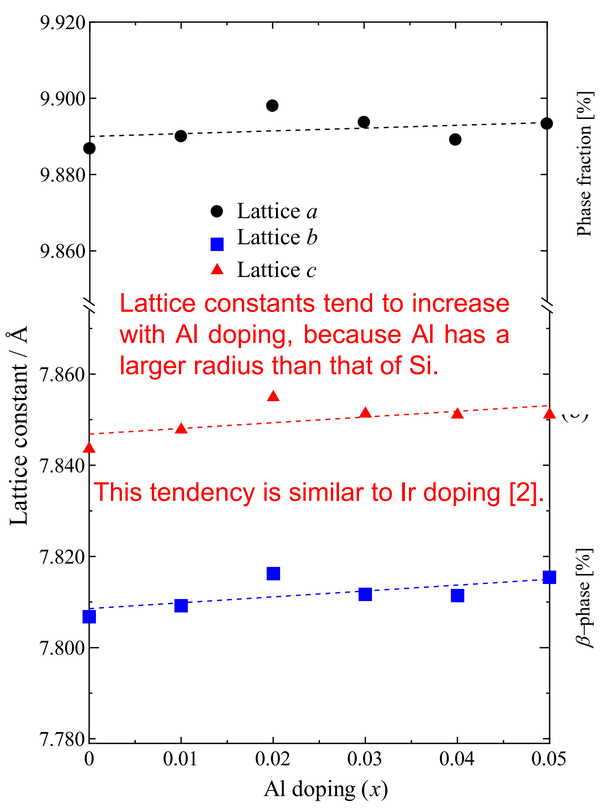
Crystal structure and microstructure of $FeSi_2$ transformation



Heat treatment is necessary to transform the metallic phases to the semiconducting phase.



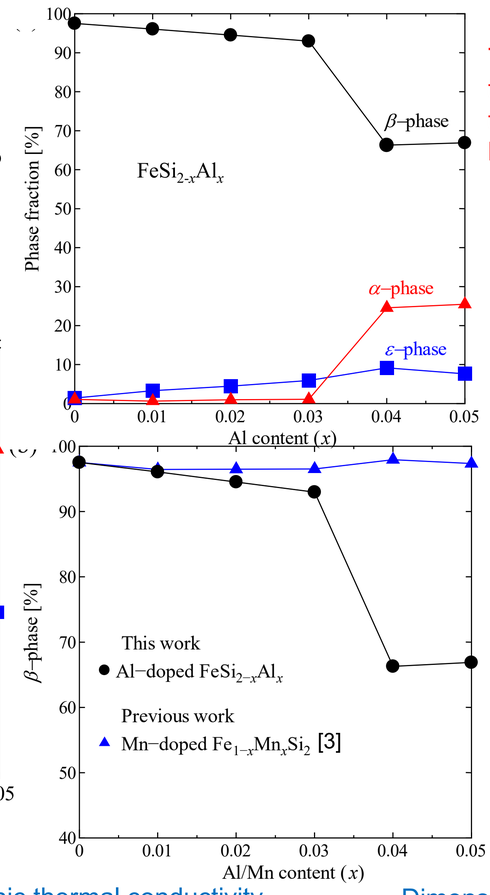
Variation in lattice constants for β-$FeSi_{2-x}Al_x$



Lattice constants tend to increase with Al doping, because Al has a larger radius than that of Si.

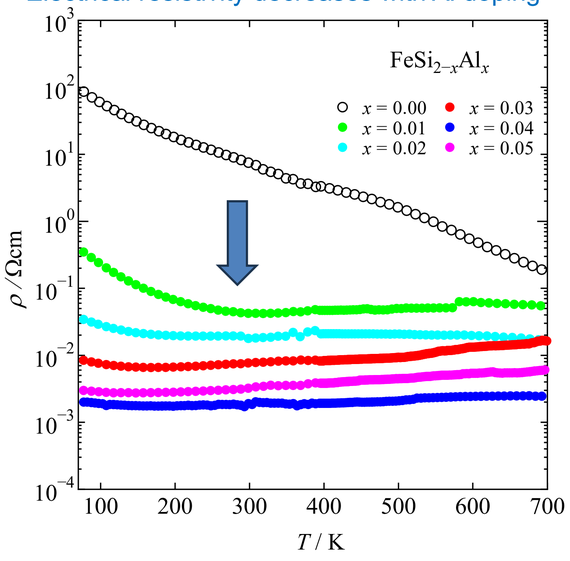
This tendency is similar to Ir doping [2].

Phase fraction analysis

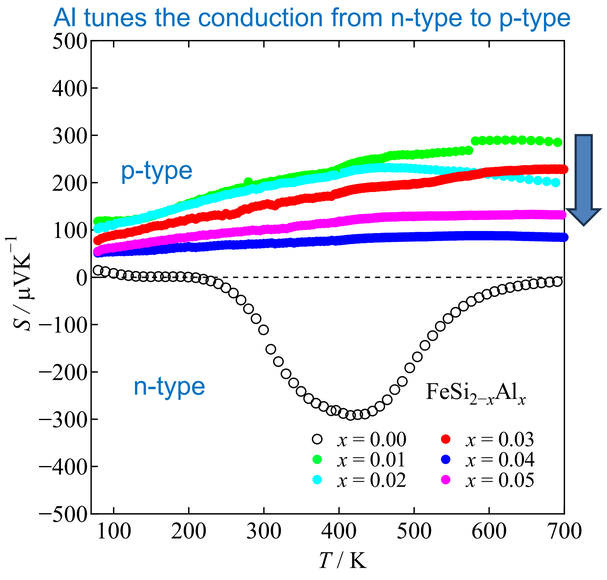


The β-phase fraction decreased markedly to below 70% at x = 0.04, indicating that the solid solubility limit of Al in β-$FeSi_2$ is lower than x = 0.04.

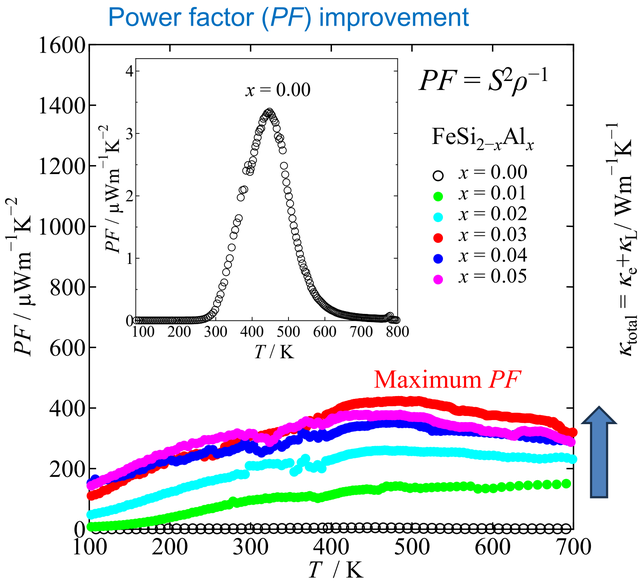
Electrical resistivity decreases with Al doping



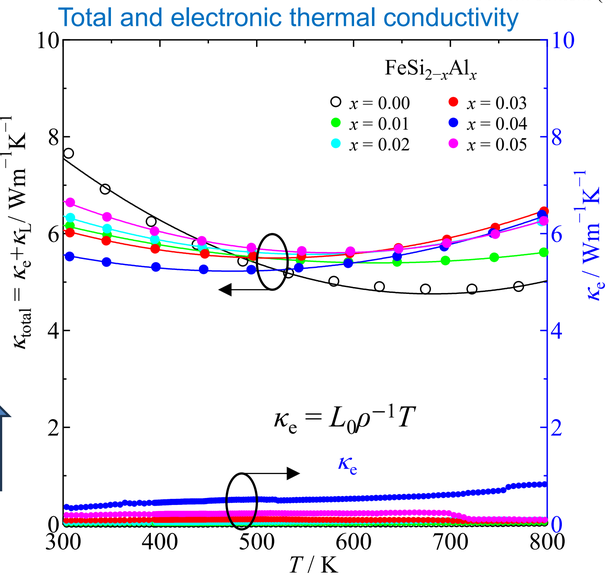
Al tunes the conduction from n-type to p-type



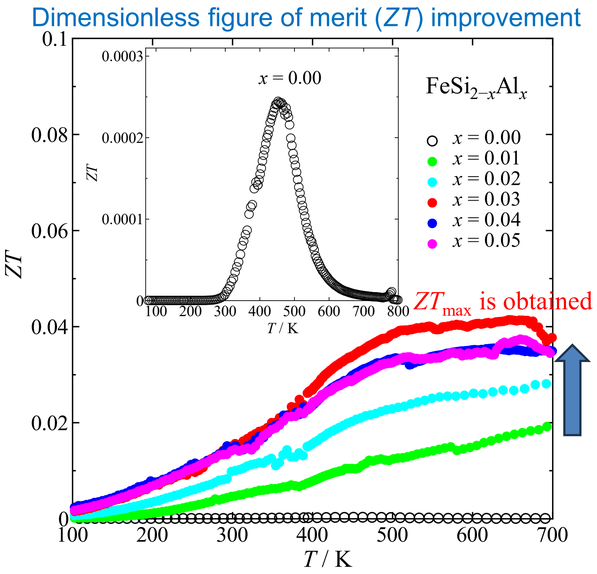
Power factor (*PF*) improvement



Total and electronic thermal conductivity



Dimensionless figure of merit (*ZT*) improvement



ZT_{max} is obtained in x = 0.03

CONCLUSIONS

- Al is incorporated into the Si sublattice, increasing the lattice constants and unit cell volume.
- The β-phase remains dominant at low Al concentrations, but significant α-phase formation at $x \geq 0.04$ indicates an Al solubility limit below $x = 0.04$ in β-$FeSi_2$.
- Al doping reduces electrical resistivity, tunes conduction from n-type to p-type, and improves the high-temperature Seebeck coefficient.
- The optimum composition is $x = 0.03$, which exhibited the highest power factor and *ZT*; thermoelectric performance is found to be strongly dependent on β-phase stability.

ACKNOWLEDGMENT/REFERENCES

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