Materialforschung durch Computer-gestützte physikalische Modellierung

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Max-Planck-Institut für Metallforschung

Gliederung

Einleitung:
theoretische Materialforschung

I. Wasserstoff in Metallen
auf interstitiellen Plätzen

Metallhydrid-Phasen: Kohäsion

H-Isotope im Metall: Vibration

II. Korngrenzen in Metallen
mit interstitiellen Fremdatomen

Segregation von B, C, N, O und H

Symmetrie und Kohäsion

Ausblick:
theoretische Energieforschung

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Zusammenarbeiten

I. Wasserstoff in Metallen

Theorie (Stuttgart)

M. Fähnle
S. Schweizer
H. Krimmel
L. Schimmele

Theorie (USA)

K. M. Ho, C. T. Chan (Ames)
J. Zhu, S. G. Louie (Berkeley)

II. Korngrenzen in Metallen

Theorie (Stuttgart, Freiburg)

R. Janisch
M. Mrovec
T. Ochs
O.Beck

Experiment (Stuttgart)

W. Sigle
W. Kurtz

Theoretical material research: energies and forces

- "Classical" atomistic modelling
  - Empirical interaction models
    - Analytical many-body potentials, ionic models, …
    - Structure optimization, molecular dynamics, Monte Carlo simulation
- Quantum mechanics, electron theory
  - Ab-initio density-functional theory
    - Pseudopotential or all-electron approaches
  - Semi-empirical tight-binding models

Materialforschung durch Computer-gestützte physikalische Modellierung

- **Mixed-basis pseudopotential method** (Meyer, Elsässer, Fähnle et al., MPI-MF Stuttgart)

- Density functional theory			local density approximations
- Translational lattice symmetry			interface supercells
- Core-valence interactions			norm-conserving pseudopotentials
- Representation of valence electrons			plane waves and localized orbitals
- Output: total energies and atomic forces		⇔	structure optimization
crystal structures and atom positions		⇔	HRTEM
electron densities and spectra		⇔	STEM-EELS
interface energies		⇔	bonding and cleavage

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⇒ Liste von Publikationen am Ende des Vortrages

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Symmetrical tilt grain boundaries in Nb and Mo

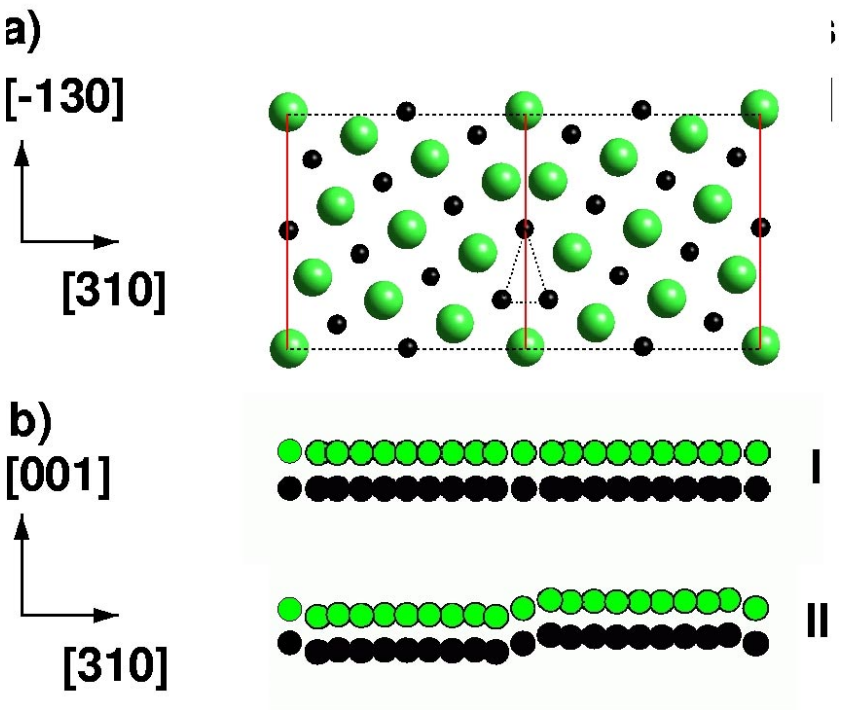
- Background: Theoretical investigation

  Translation states of twins in pure bcc metals

  LDFT of the Σ5 (310) [001] STGB

  ⇒ T.Ochs et al., Phil. Mag. A 80 (2000) 351

	valence electons	$\Delta\sigma$ mJ/m^2	$\Delta\tau$ % of a_0
Nb	$4d^4\,5s^1$	8	8
Mo	$4d^5\,5s^1$	108	18
Ta	$5d^3\,6s^2$	0	0
W	$5d^4\,6s^1$	100	20



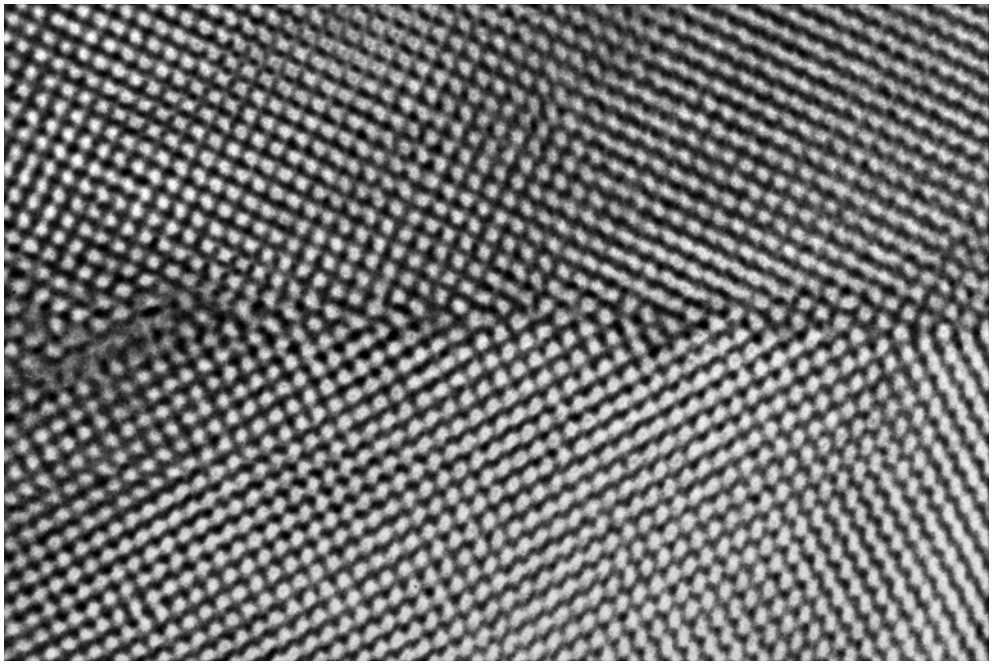
⇒ Translation state depends on valence configuration

- Experimental observations

HRTEM of the Σ5 (310) [001] STGB

- In Nb, Mo, Ta by G. Campbell et al. (1993, 1999, 2000)
- In Mo by W. Sigle (2001)

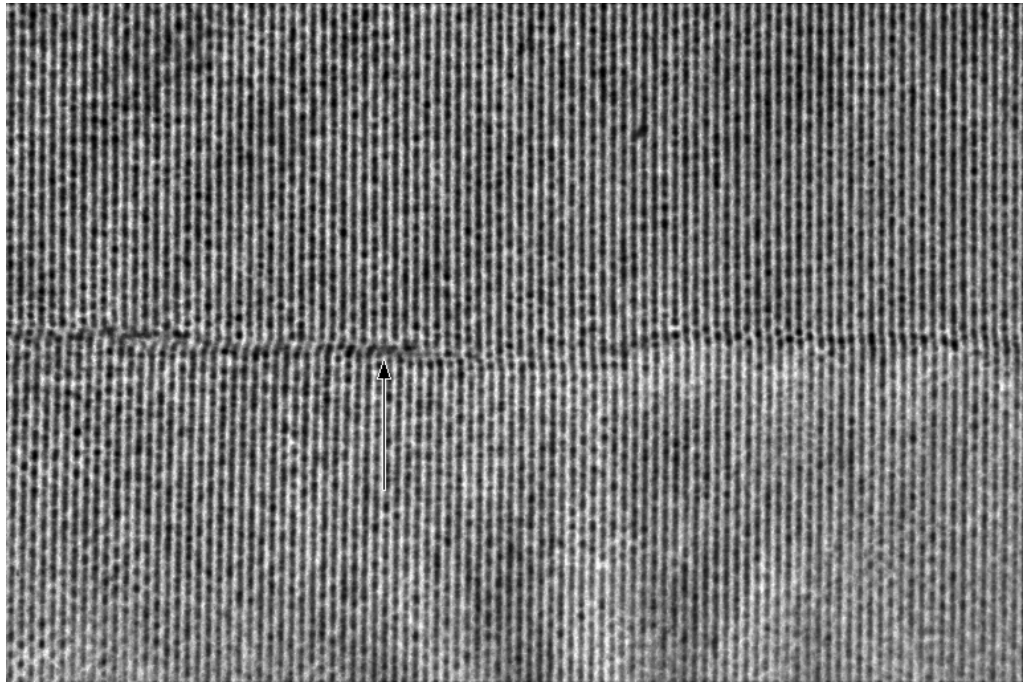
HRTEM image along the [001] zone axis



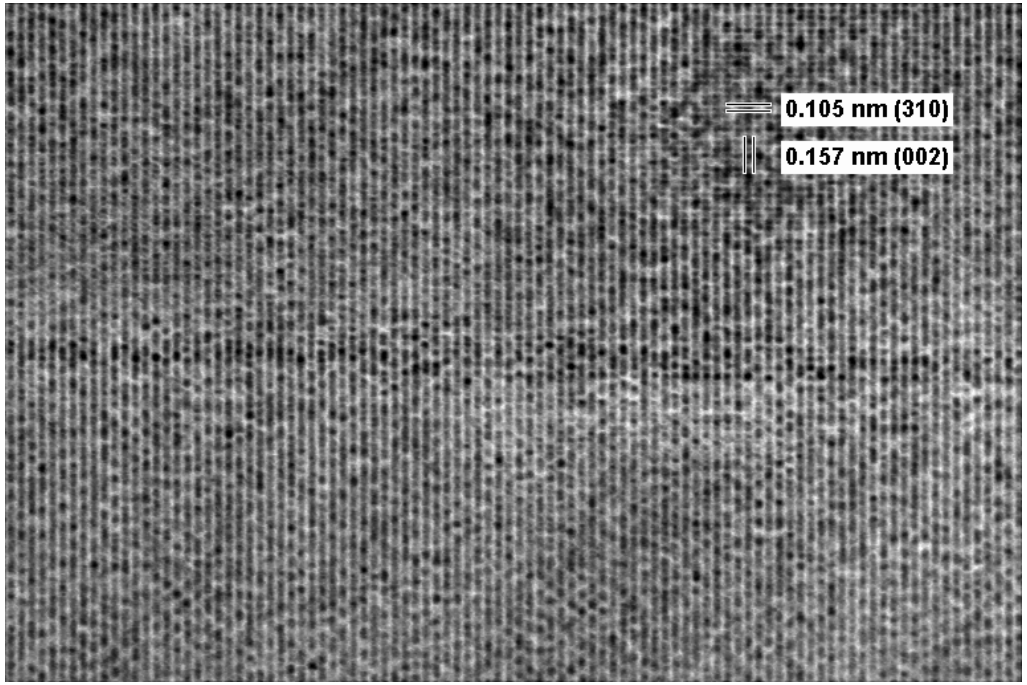
W. Sigle, MPI-MF Stuttgart (2001)

- Experimental observations for Mo

HRTEM images along the [-130] axis



W. Sigle, MPI-MF Stuttgart (2001)



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⇒ [Influence of structural imperfections?]

⇒ Influence of segregated impurities?

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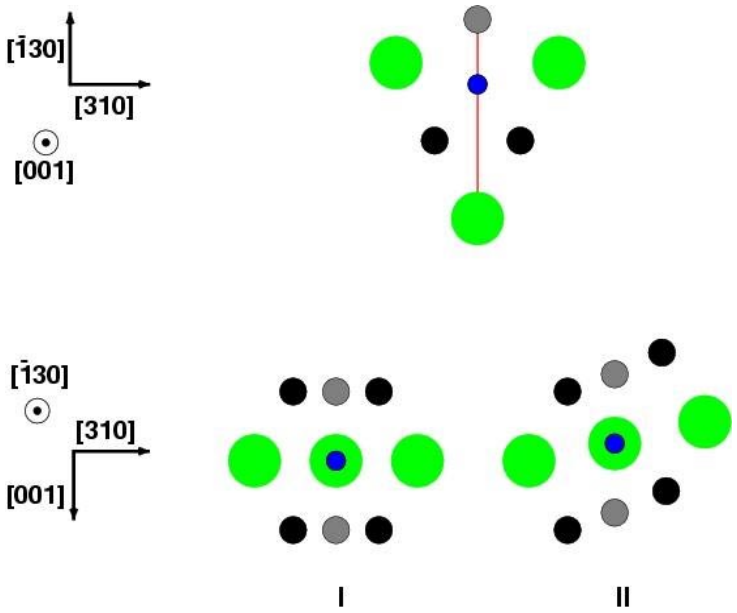
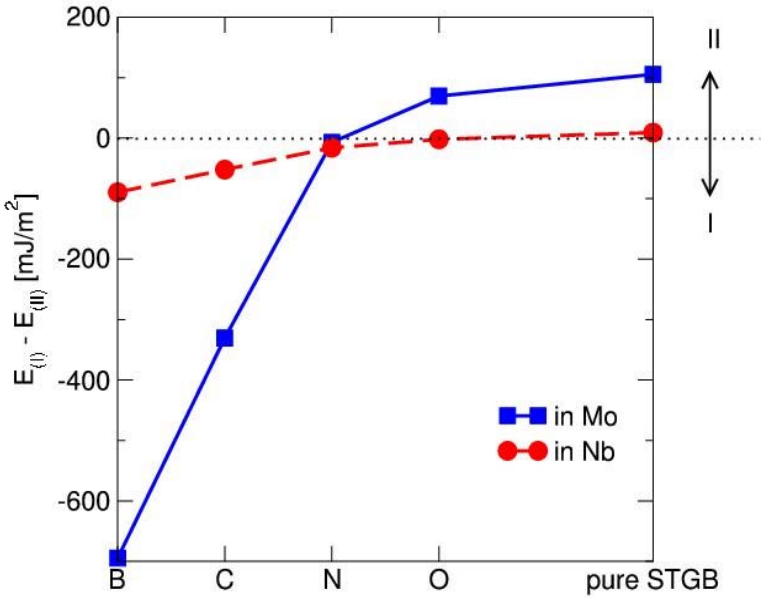
- Theoretical analysis

insert impurity atoms at GB sites



GB energy differences



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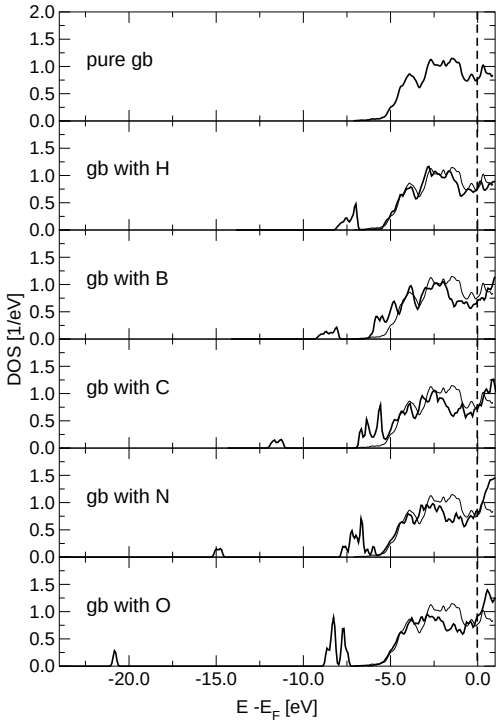
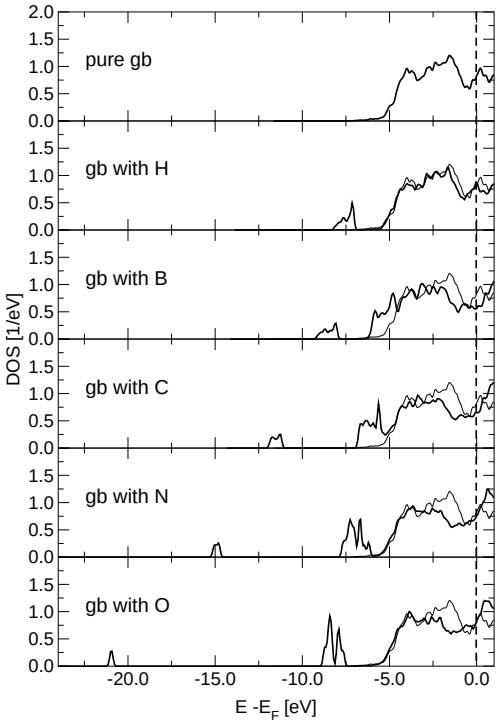
Site-projected densities of electron states at the GB

Nb



Mo



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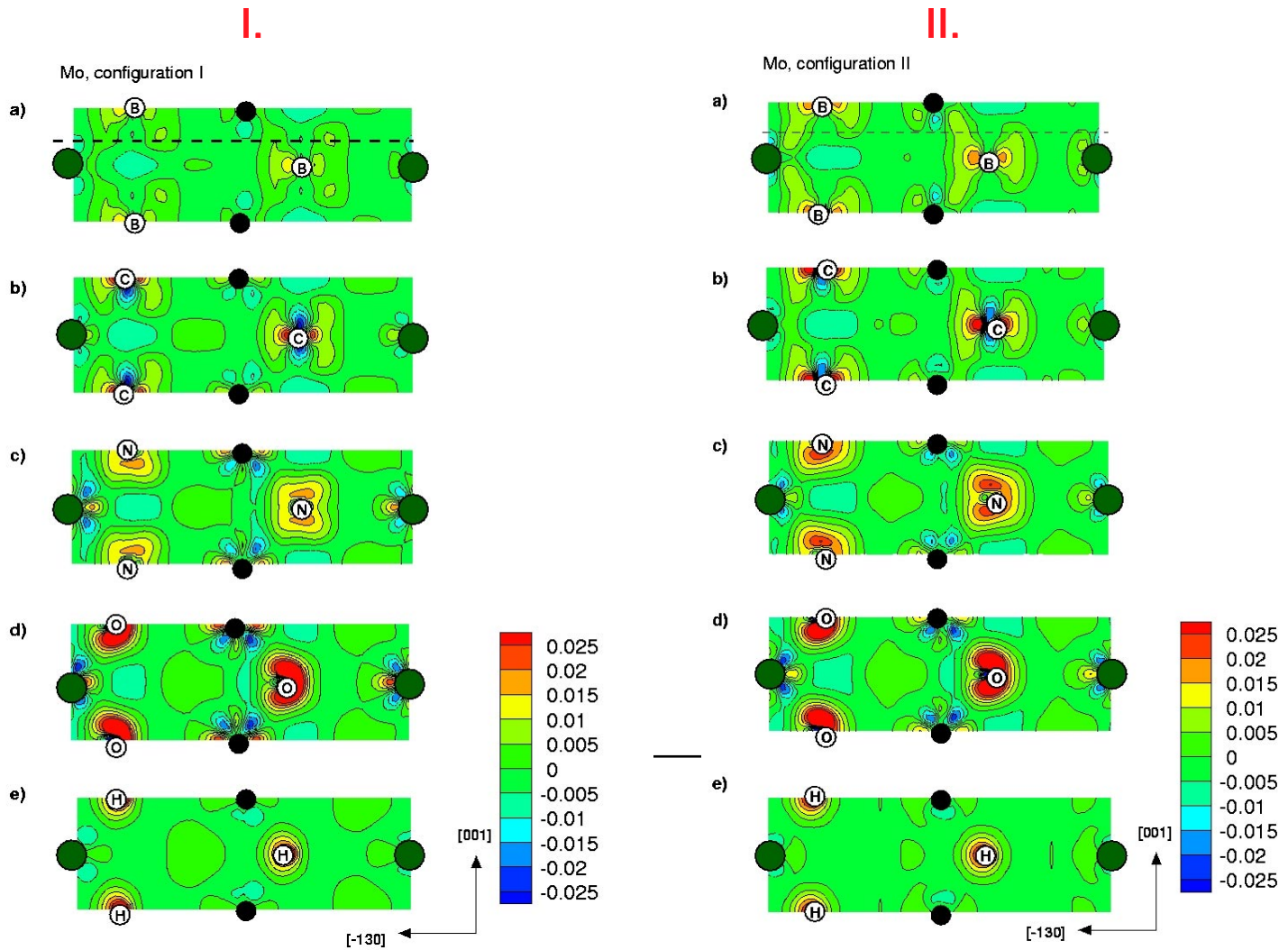
Bonding electron densities along the GB plane in Mo



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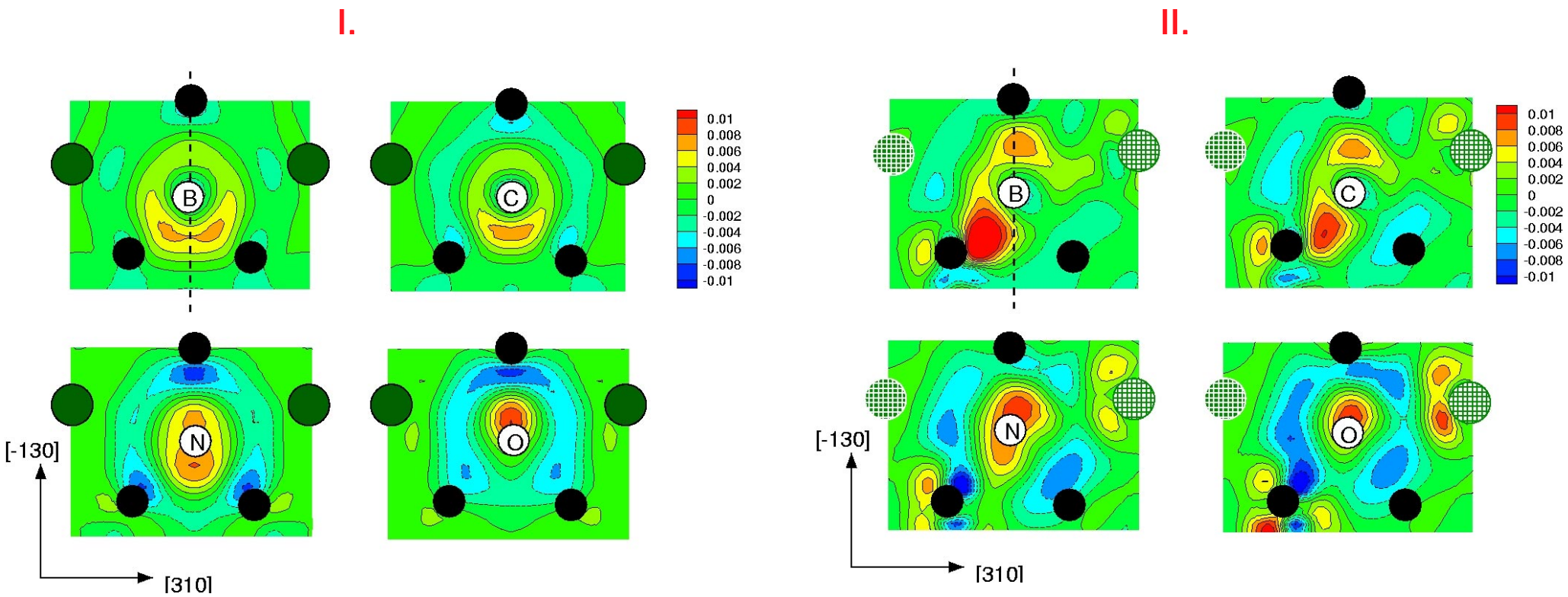

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- Theoretical interpretations

Bonding energies ΔE_B of the impurities

- **Cottrell**, Mater. Sci. Technol. 6 (1990) 807: hybridization vs. embedding
  - Covalently bonding atoms increase GB cohesion
  - Polarly bonding atoms enhance GB brittleness

- **Rice and Wang**, Mater. Sci. Engr. A 107 (1989) 23: boundary vs. surface
  - $\Delta E_B = E_B^{GB} - E_B^{FS}$

LDFT	B	C	N	O
ΔE_B in J/m^2	1.08	0.31	-0.81	-1.46

- Conclusions

  Σ5 (310) [001] STGB in Nb & Mo

  - B and C — form covalent bonds with the host metal; stabilize mirror-symmetric GB configuration I; increase GB cohesion
  - N and O — form polar bonds with the host metal; stabilize symmetry-broken GB configuration II; enhance GB brittleness

⇒ R. Janisch and C. Elsässer,

Phys. Rev. B **67** (2003) 224101

Theoretical energy research: predictive power

- Calculation of physical properties
  - Atomistic structures: lattice parameters, atom positions
  - Electronic states: electron densities, electron spectra
  - Properties of materials: mechanical, chemical, thermal, electric, magnetic, optical, ...

- Analysis of chemical bonds
  - Metallic screening, covalency and polarity, ionic charge transfer
  - Empirical many-body potentials from ab-initio results

Publikationen

I. Wasserstoff in Metallen

PdH	C. E. et al., Phys. Rev. B 44 (1991) 10377
ZrH_2	C. E. et al., MRS Symp. Proc. Vol. 453 (1997) 221
NiH, FeH	C. E. et al., J. Phys.: Condens. Matter 10 (1998) 5081, 5113, 5131

II. Korngrenzen in Metallen

perfekt reine Σ5-KG in Nb und Mo
T. Ochs et al. Phil. Mag. A 80 (2000) 351, 2405

Σ5-KG in Nb und Mo mit segregiertem B, C, N, O und H
R. Janisch und C.E., Phys. Rev. B 67 (2003) 224101

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„Energieforschung“

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