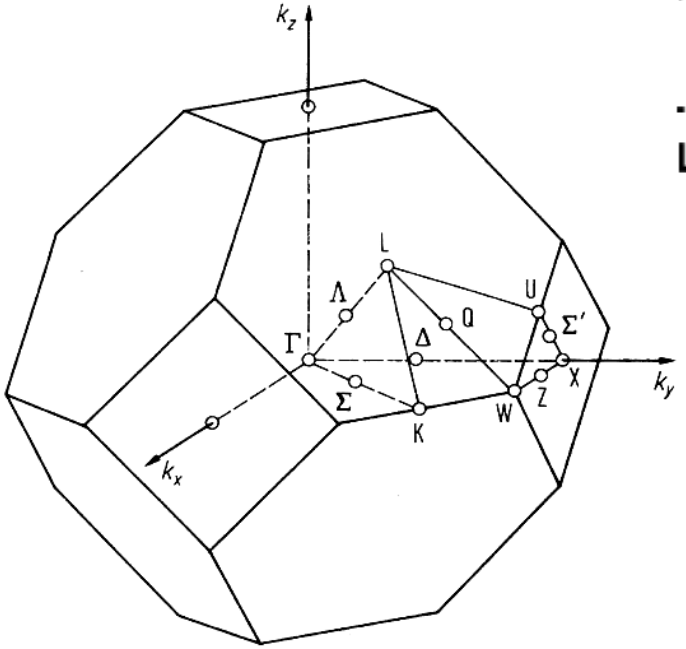
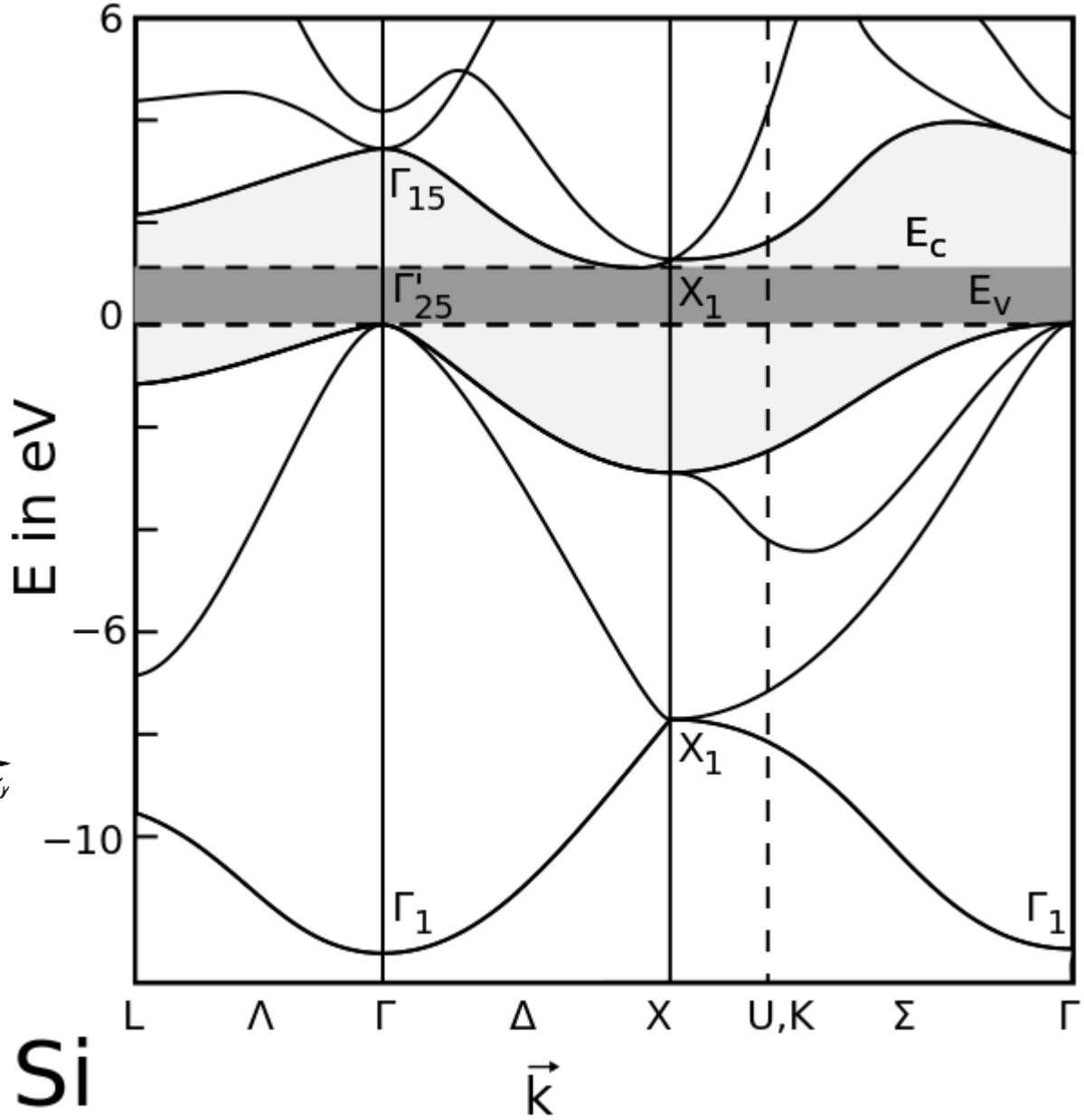
technische universität
dortmund

Materialklassen

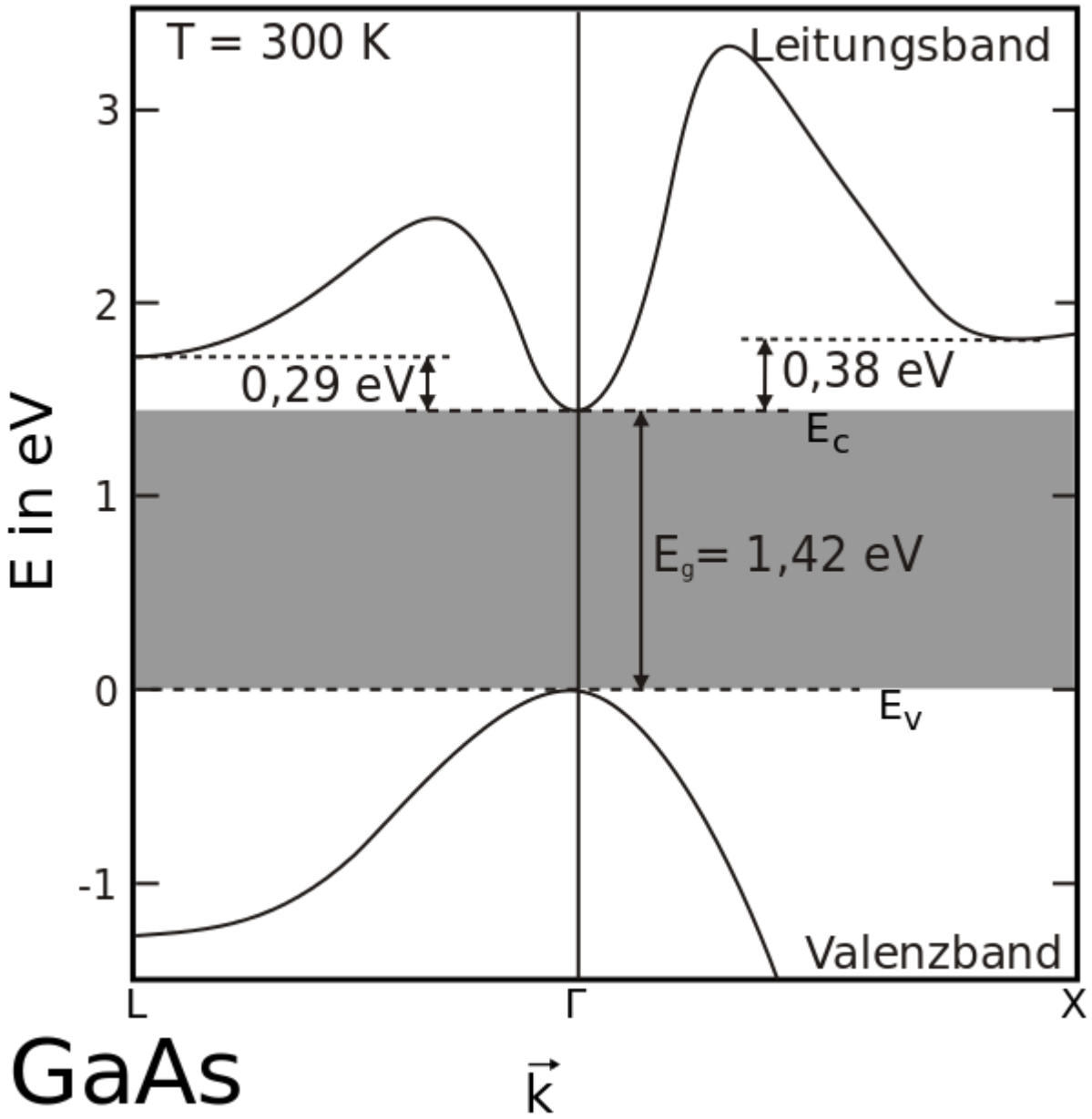
Bandstrukturen:

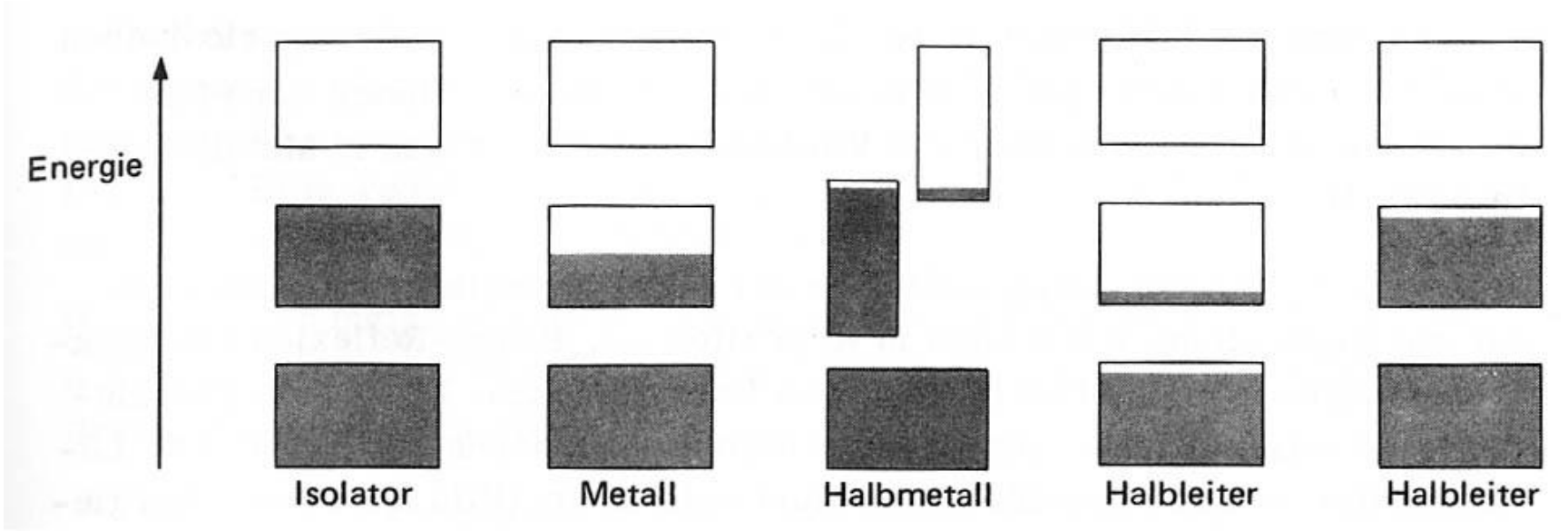




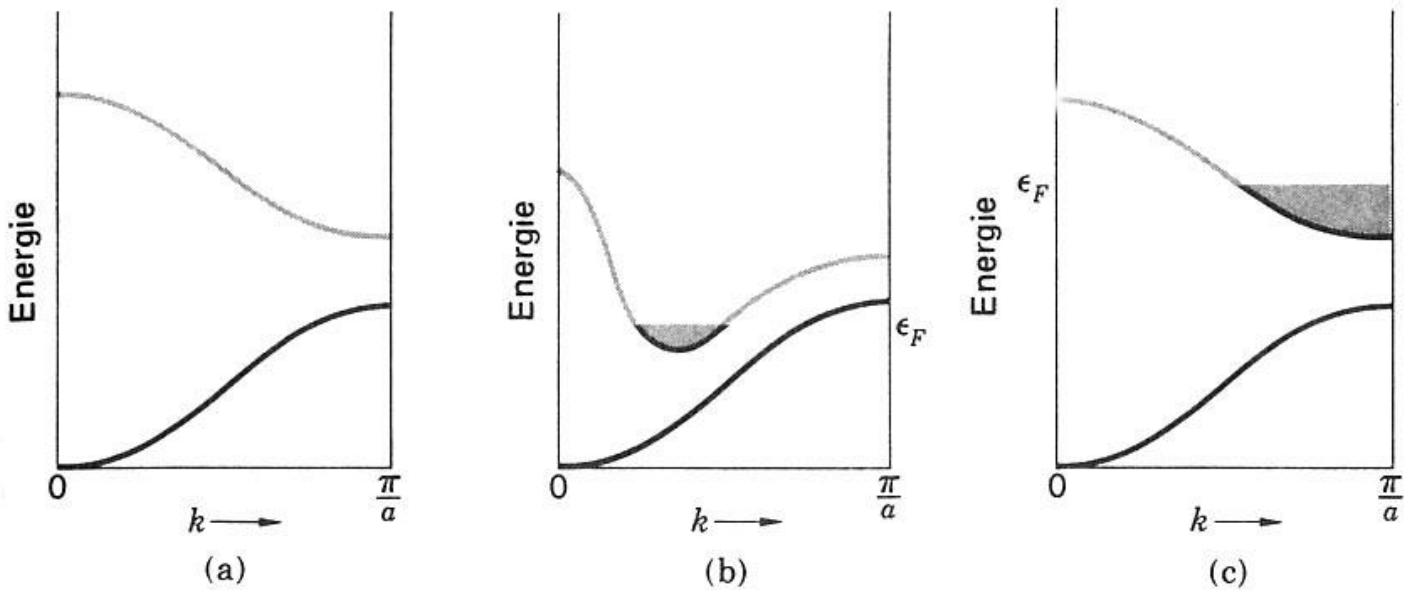
Si

Bandstrukturen:





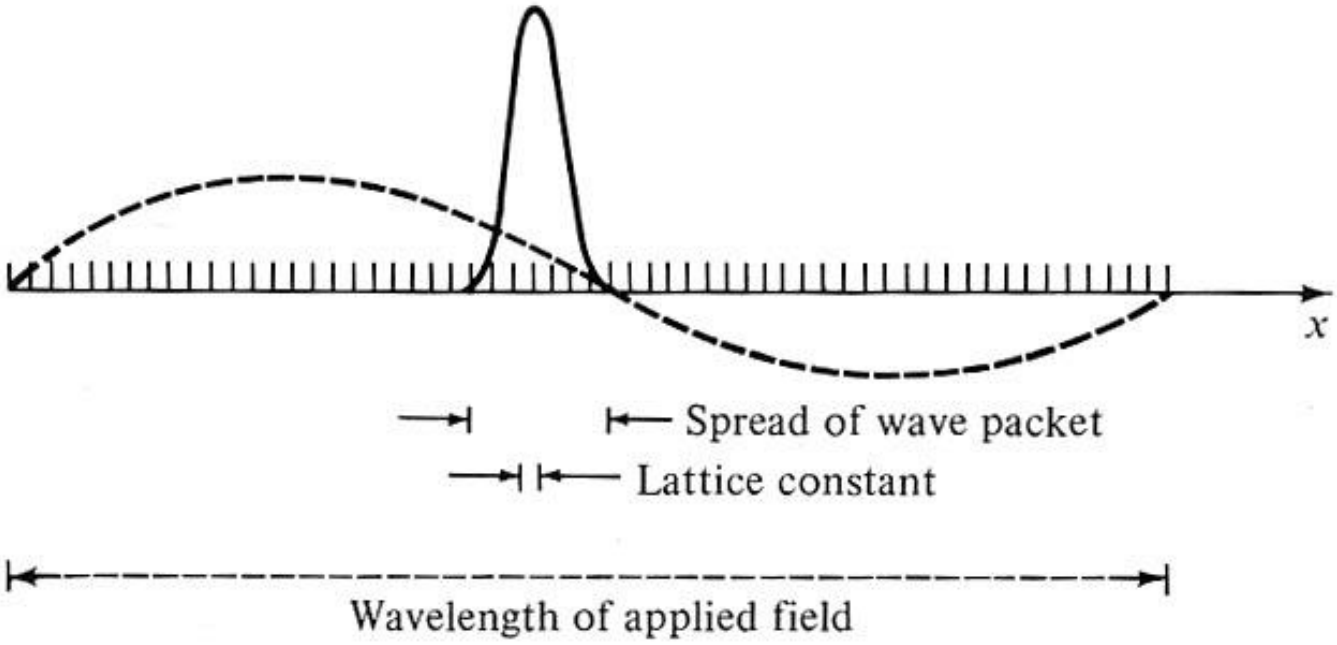
Unterschiedliche Besetzung der Bänder mit Elektronen (Ortsraum)



Unterschiedliche Besetzung der Bänder mit Elektronen
(Reziproker Raum)

Hamiltonian für Wechselwirkung mit Phononen

$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N}} \sum_{\substack{\vec{k},\vec{G},\vec{q},\\ j,b,b',\sigma}} v_{\vec{k},\vec{G},\vec{q};j,b,b'} \left(b^{\dagger}_{j,-\vec{q}} + b_{j\vec{q}} \right) c^{\dagger}_{b,\vec{k}+\vec{q}+\vec{G},\sigma} c_{b',\vec{k},\sigma}$$



Begründung des semiklassischen Modells

COMPARISON OF SOMMERFELD AND BLOCH ONE-ELECTRON EQUILIBRIUM LEVELS

	SOMMERFELD	BLOCH
QUANTUM NUMBERS (EXCLUDING SPIN)	$\mathbf{k}$ ($\hbar\mathbf{k}$ is the momentum.)	$\mathbf{k}$, n ($\hbar\mathbf{k}$ is the crystal momentum and n is the band index.)
RANGE OF QUANTUM NUMBERS	$\mathbf{k}$ runs through all of k-space consistent with the Born-von Karman periodic boundary condition.	For each n, $\mathbf{k}$ runs through all wave vectors in a single primitive cell of the reciprocal lattice consistent with the Born-von Karman periodic boundary condition; n runs through an infinite set of discrete values.
ENERGY	$\mathcal{E}(\mathbf{k}) = \dfrac{\hbar^2 k^2}{2m}$.	For a given band index n, $\mathcal{E}_n(\mathbf{k})$ has no simple explicit form. The only general property is periodicity in the reciprocal lattice: $\mathcal{E}_n(\mathbf{k} + \mathbf{K}) = \mathcal{E}_n(\mathbf{k})$.
VELOCITY	The mean velocity of an electron in a level with wave vector $\mathbf{k}$ is: $\mathbf{v} = \dfrac{\hbar\mathbf{k}}{m} = \dfrac{1}{\hbar}\dfrac{\partial\mathcal{E}}{\partial\mathbf{k}}$.	The mean velocity of an electron in a level with band index n and wave vector $\mathbf{k}$ is: $\mathbf{v}_n(\mathbf{k}) = \dfrac{1}{\hbar}\dfrac{\partial\mathcal{E}_n(\mathbf{k})}{\partial\mathbf{k}}$.
WAVE FUNCTION	The wave function of an electron with wave vector $\mathbf{k}$ is: $\psi_{\mathbf{k}}(\mathbf{r}) = \dfrac{e^{i\mathbf{k}\cdot\mathbf{r}}}{V^{1/2}}$.	The wave function of an electron with band index n and wave vector $\mathbf{k}$ is: $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$ where the function $u_{n\mathbf{k}}$ has no simple explicit form. The only general property is periodicity in the direct lattice: $u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$.