Effect of dielectric mismatch on transport in Nanostructures

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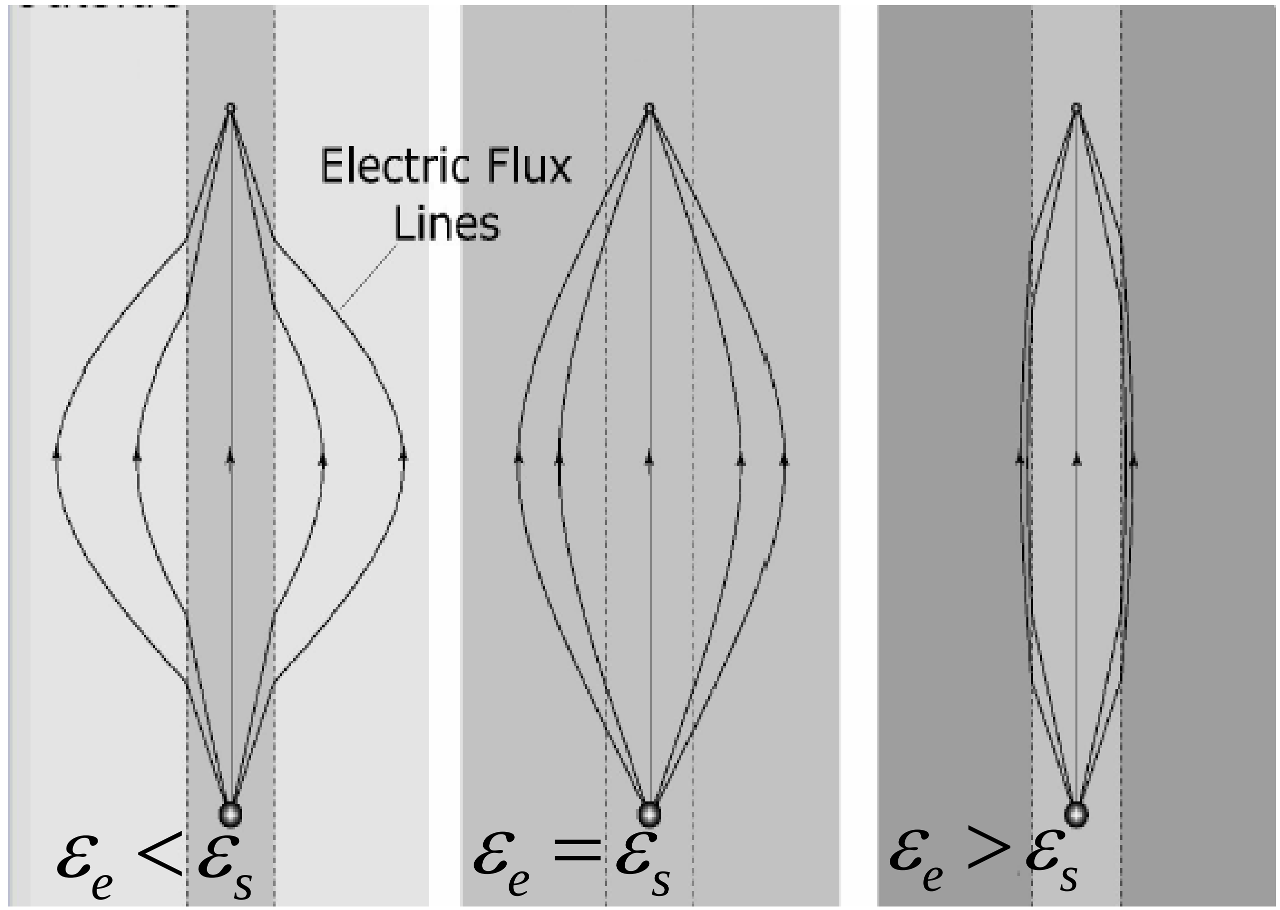
2D Dielectric mismatched structure

- Modulated by environmental dielectrics:
  - Optical properties- excitonic binding energy
  - Electrical properties- Coulombic scattering- Mobility

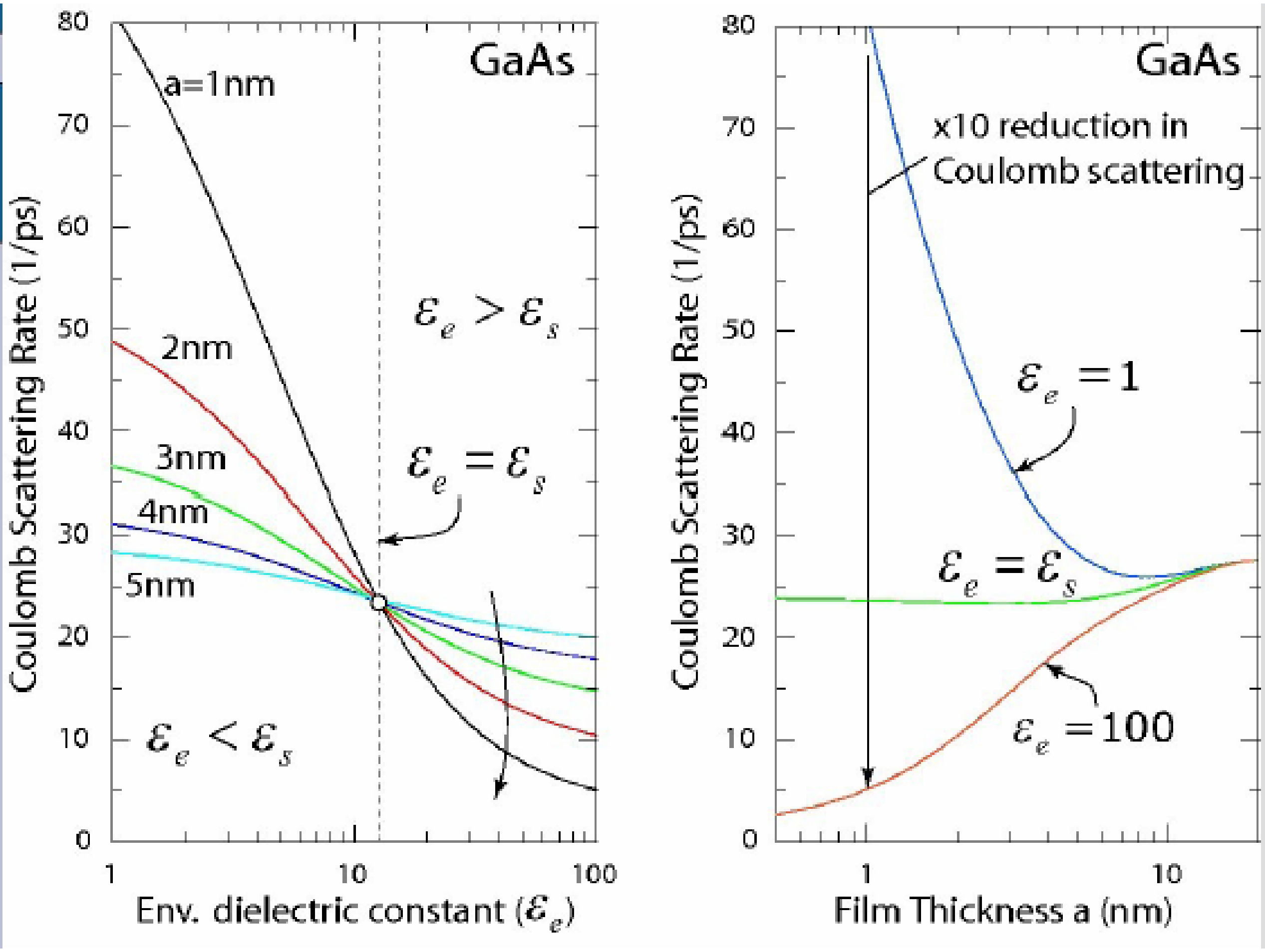


$$V(z) \sim \frac{e^2}{4\pi\varepsilon_s z} \quad \xrightarrow{\text{Long wave length limit}} \quad V(z) \sim \frac{e^2}{4\pi\varepsilon_e z}$$

← Homogeneous bulk material

1. D. Jena et al. (communicated to Phys. Rev. Lett.)
2. L.V. Keldysh, “Coulomb interaction in thin semiconductor and semimetal films,” JETP Lett., vol. 92, p.658, 1979

Motivation



- Mobility determined by scattering mechanism:
  - Coulombic Scattering
  - Surface Roughness Scattering
  - Phonon Scattering
- Two parameters to tune the Coulombic Scattering rate:
  - Thickness of semiconductor
  - Environmental dielectric constant
- SR scattering mechanism

1. M.Kumagai et al., Phys. Rev. B 40,12359
2. R.E. Prange et al., Phys Rev. 168, 779
3. H. Sakaki et al., Appl. Phys. Lett. 51, 1934

Coulombic Scattering rate calculation

- Tools:
  - Green's Function solution of Poisson equation
  - Theory of Image charges
- Unscreened Coulombic scattering potential (modulated by environmental dielectric):

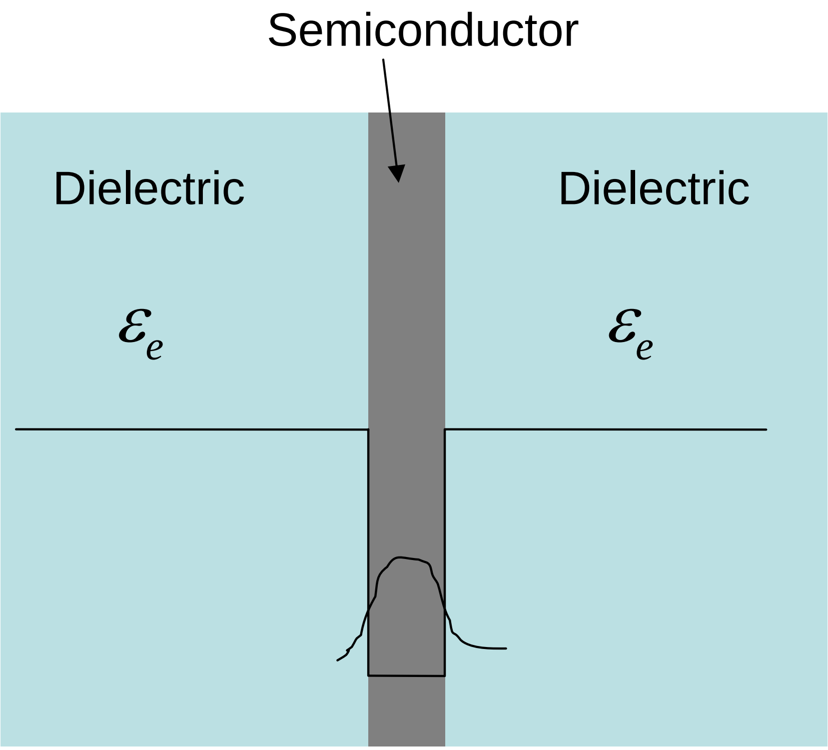
$$V(\vec{\rho}, z) = \sum_{-\infty}^{\infty} \frac{e\gamma^{|n|}}{4\pi\varepsilon_0\varepsilon_s\sqrt{|\vec{\rho}|^2 + |z - z_0|^2}} \quad \text{, where} \quad \gamma = \frac{\varepsilon_s - \varepsilon_e}{\varepsilon_s + \varepsilon_e}$$

- Envelope function of 2D dielectric mismatched structure:

$$\Psi_{n_z, k_{//}} = \sqrt{\frac{2}{W}} \cos\left(\frac{n_z \pi z}{W}\right) \frac{1}{\sqrt{L_x L_y}} e^{i(\vec{k} \bullet \vec{\rho})}$$

- Matrix element of scattering potential: $H^{a,e}_{k',k} = \frac{1}{A}\int \Psi^*_{1,k'} V(\vec{\rho}, z) \Psi_{1,k} dA$
- Scattering rate calculation: Fermi's Golden Rule

Problem we want to address



- The potential barrier is finite
- The electron wave function leaks into dielectrics, changing its effective mass
- Estimation of critical band offset for good confinement of electrons
- For different materials: role of effective mass/band gap in mobility calculation
- Polarization sources
    - Electronic polarization
    - Ionic polarization