Resistivity-film thickness model using surface scattering model and van der Pauw method of measuring resistivity.

Group meeting (06/04/2021)

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Scattering of conduction electrons

- Scattering of conduction electrons reduce mean free path
- Scattering from surfaces, grain boundaries, rough surfaces, impurities

t: film thickness

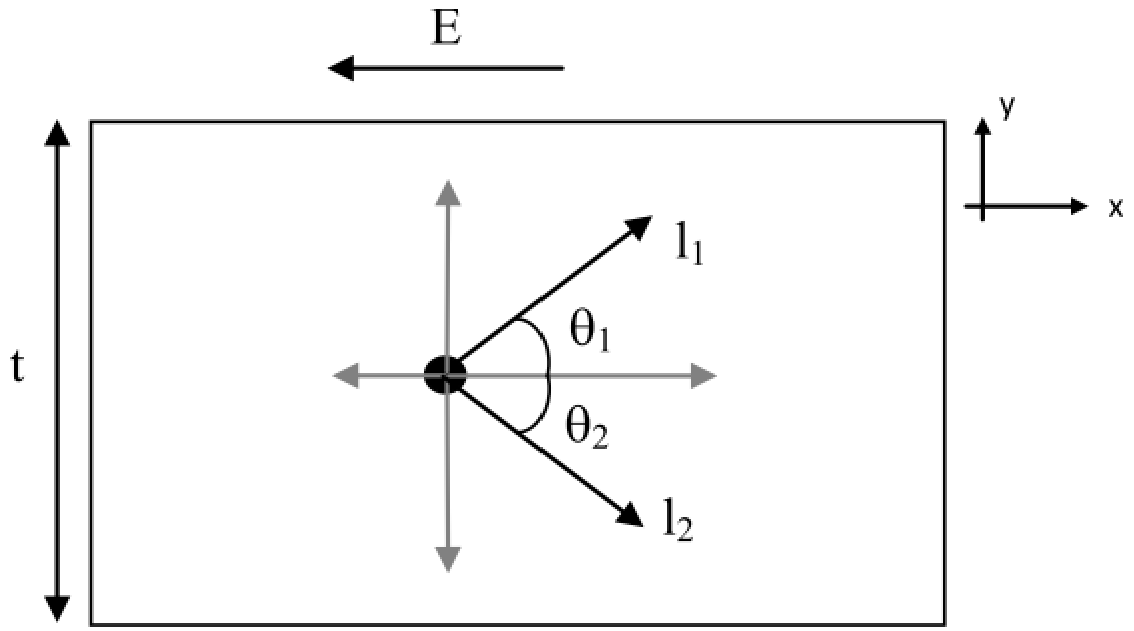
l : mean free path

$\rho = \rho_0$ bulk resistivity

$$l_{film} = \beta l_{bulk}$$

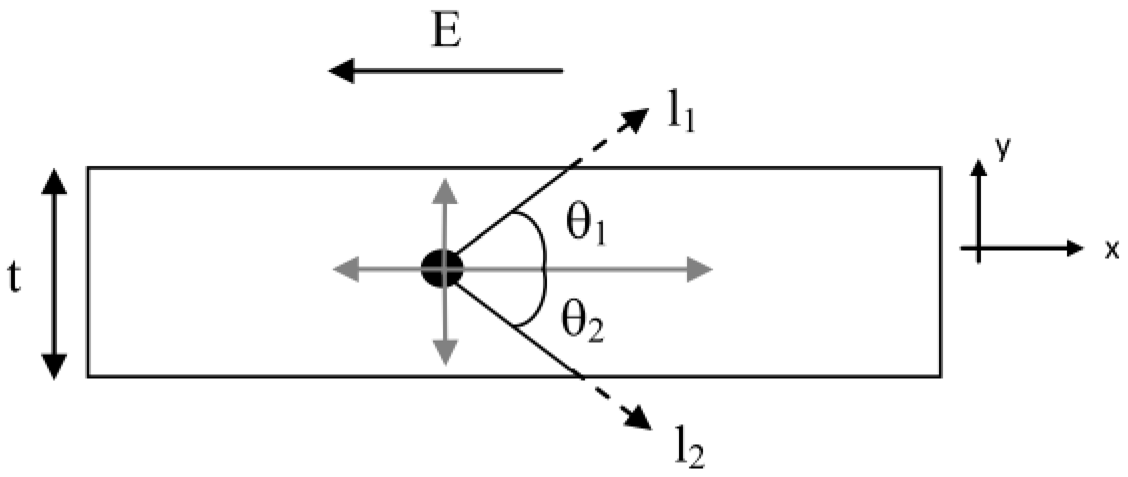
Case I

$$l_1 = l_2 < \frac{t}{2}$$



Case II

$$l_1 = l_2 > \frac{t}{2}$$



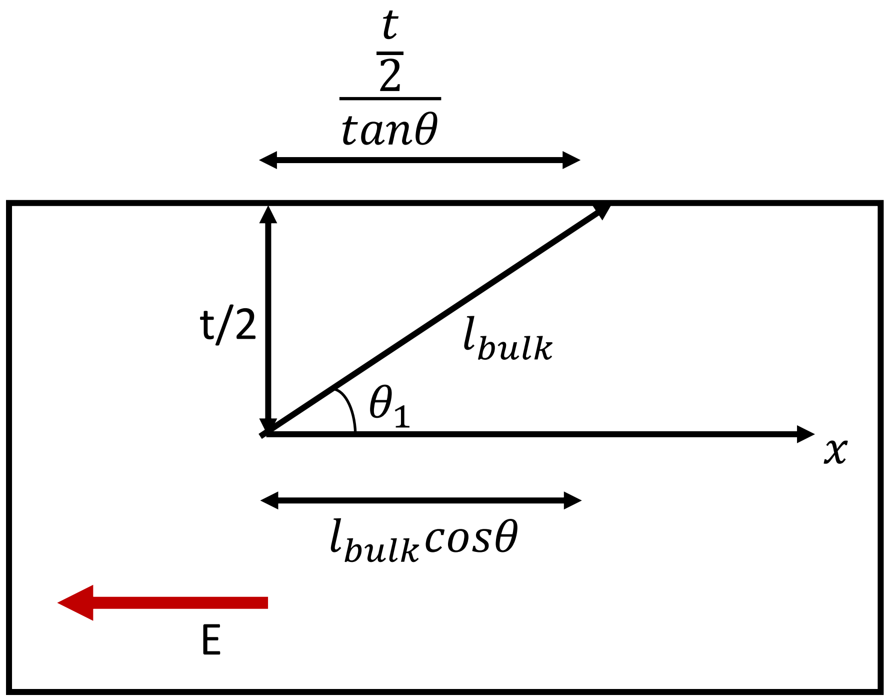
Derivation

For second case $\left(l_1 = l_2 > \frac{t}{2}\right)$,

$\theta_1 = \sin^{-1}\frac{\frac{t}{2}}{l_{bulk}}$,

For $\theta_1 > \theta$, Propagation in x-direction $l_{bulk}\cos\theta$

For $\theta_1 < \theta$, Propagation in x-direction is $\frac{\frac{t}{2}}{tan\theta}$



$$\beta = \frac{\frac{2}{\pi}\left[\int_0^{\sin^{-1}\frac{\frac{t}{2}}{l_{bulk}}} l_{bulk}cos\theta d\theta + \int_{\sin^{-1}\frac{\frac{t}{2}}{l_{bulk}}}^{\frac{\pi}{2}} \frac{\frac{t}{2}}{tan\theta} d\theta\right]}{\frac{2}{\pi}\int_0^{\frac{\pi}{2}} l_{bulk}cos\theta d\theta}$$

$$= \frac{t}{2l_{bulk}}\left[1 - \ln\frac{\frac{t}{2}}{l_{bulk}}\right] = \kappa[1 - \ln\kappa]$$

$$Where, \kappa = \frac{t}{2l_{bulk}}$$

$$\rho = \frac{m}{ne^2\tau} \; and \; \tau = \frac{l}{v_F}$$

$$\rho_{film} = \frac{\rho_0}{\kappa[1 - \ln\kappa]}$$

For $\kappa < 1, \rho > \rho_0$

Additional scattering effects:

- Additional scattering further reduce the mean free length and increase resistivity
- Impurity concentration, processing techniques has larger effect on bulk resistivity
- Grain boundary size and rough surface are more prominent for smaller film thickness

- Resistivity larger than ρ_0 when thickness larger than twice of mean free path means the increased resistivity is because of processing technique as well as impurities

$$\rho_0' = c\rho_0, \text{ where scaling factor c > 1}$$

- Scattering from grain boundary and rough surfaces (<20nm) reduce the effective thickness giving

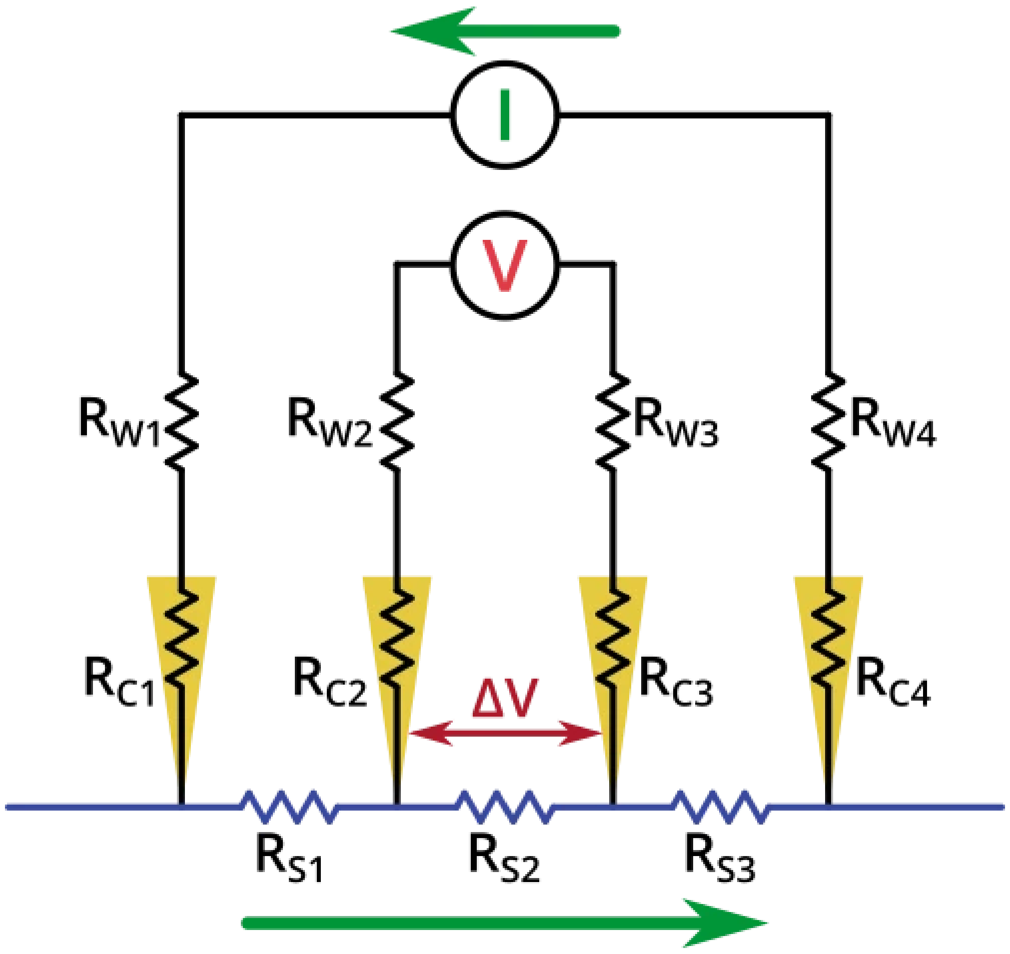
$$\kappa' = \frac{t - \eta}{2 l_{bulk}}$$

- Thus, resistivity of thin film becomes

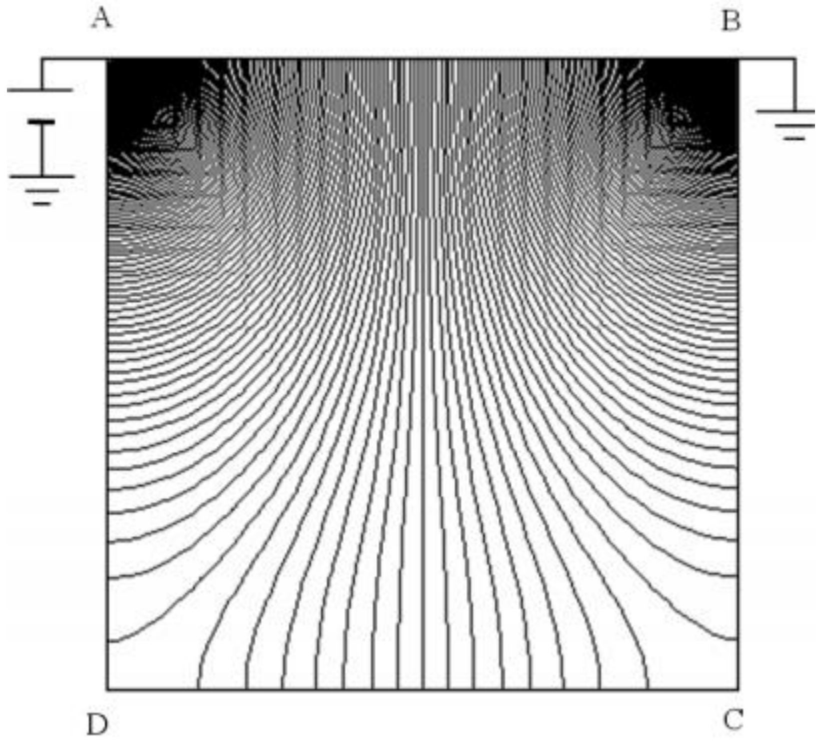
$$\rho' = \frac{c\rho_0}{\kappa'[1 - \ln \kappa']}$$

Van der Pauw method:

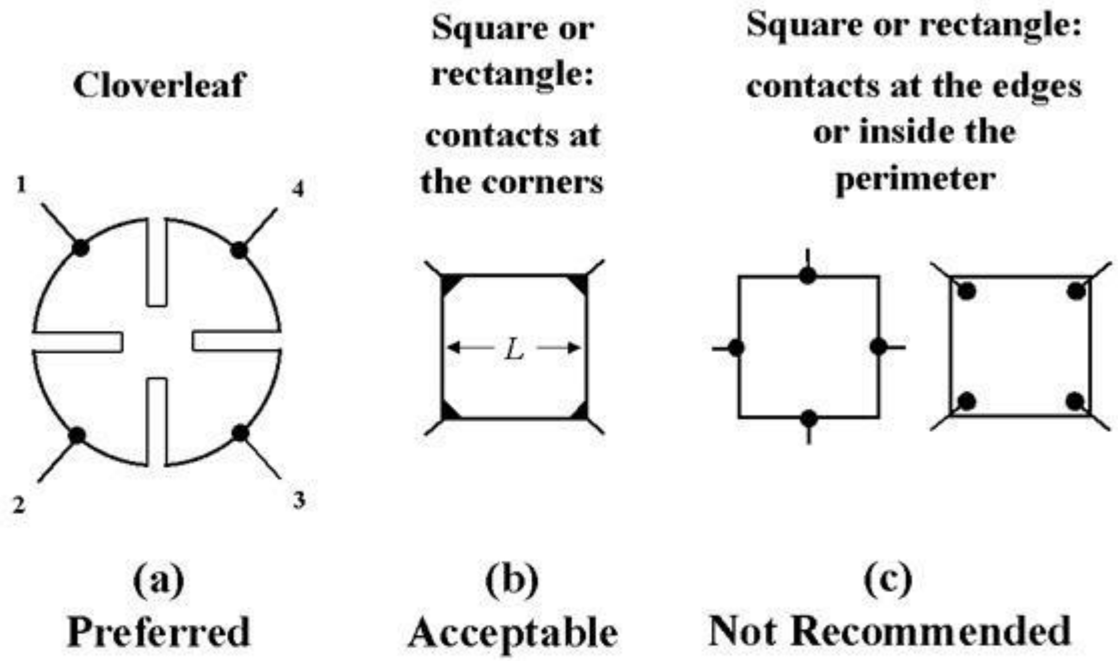
Four-point method to remove contact resistance



Equipotential lines because of current through one edge

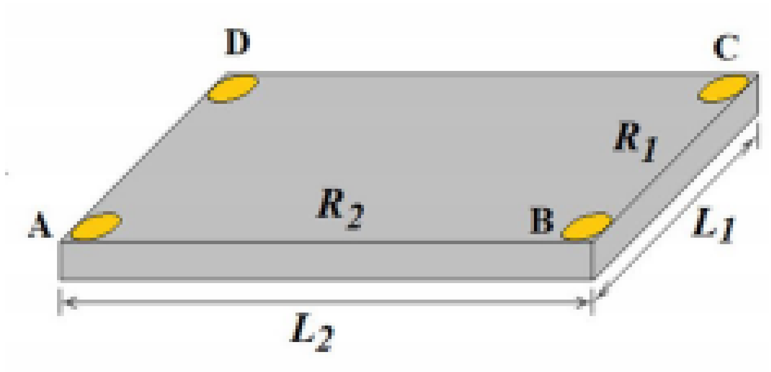


Conditions required:



Ref. Wikipedia

- The sample must have a flat shape of uniform thickness
- The sample must not have any isolated holes
- The sample must be homogenous and isotropic
- All four contacts must be located at the edges of the sample
- The average diameters (D) of the contacts, and sample thickness (t) must be much smaller than the distance between the contacts (L).
- Relative errors caused by non-zero values of D are of the order of D/L



$$R_1 = \frac{V_{CD}}{I_{AB}} \ or \ \frac{V_{AB}}{I_{CD}} \ (Vertical)$$
$$R_2 (Horizontal)$$

R_1 and R_2 are average of different combination by reversing polarity.
Helps to increase accuracy by cancelling thermoelectric potential

Van der Pauw formula for arbitrary shape of sample:

$$e^{-\frac{\pi R_1}{R_S}} + e^{-\frac{\pi R_2}{R_S}} = 1$$
$$R_S: Sheet\ resistance$$

Can be solved for R_S numerically.

Resistivity $(\rho) = R_S t$

For square shape sample where $R_1 = R_2 = R$,

$$R_S = \frac{\pi R}{ln2}$$

Conclusion:

- Resistivity of thin film goes up as the sample gets thinner.
- Resistivity of thin film can be measured by using van der Pauw method with more accuracy.

Thank you!

- Scattering by rough surface and grain boundary
- E -> x, grain boundaries yz plane, represented by series of delta function located at x_n with strength S_MS

$$\rho = \frac{\pi d}{\ln 2}\left(\frac{R_1 + R_2}{2}\right) f(R_1/R_2),$$

$$\cosh\left(\left[\frac{x-1}{x+1}\right]\frac{\ln 2}{f}\right) = \frac{1}{2}\exp\left(\frac{\ln 2}{f}\right).$$

$\rho = \rho_t + \rho_i$ Phonon(temperature dependent) +imperfection
Matthienssen's rule
Temperature dependent part electron-phonon interaction(Bloch and Gruneisen) linear at high temperature
Not valid for low temperature -> lattice imperfection includes surfaces and grain boundaries -> mean free path-> T dependent

Model
Mayadas and Shatzkes(assumption)

- Semiclassical transport between grain boundaries
- Grain boundaries are perpendicular to transport
- Grain boundaries are translation-invariant along the boundary
- Transmission can be characterized by parameter R
- All boundaries in a sample are identical

Other sophisticated model don't combine the influence of grain boundary and surface
Temperature is not explicit variable but incorporated with mean free path-> doesnot have simple form-> no analytical relation

$$\frac{\rho_B}{\rho_g} = f(\alpha)$$

$$f(\alpha) = 1 - \frac{3}{2}\alpha + 3\alpha^2 - 3\alpha^3 \ln\left(1 + \frac{1}{\alpha}\right)$$

$$\alpha = \frac{\lambda_B}{D}\frac{R}{1-R}; D \rightarrow radius\ of\ grain, R \rightarrow grain\ boundary\ reflection\ coefficient$$

$$\frac{\rho_B}{\rho_f} = f(\alpha) - g(k, p, \alpha)$$

Van der Pauw method of measuring resistivity

- Sample thickness much smaller than width and length
- $\rho = R_s t$ (Isotropic)
- Arbitrary shape
- Switching polarity helps to cancel thermoelectric potential due to Seebeck effect

- With regard to the physical properties, measuring electrical conductivity is of great relevance for understanding several physical phenomena such as superconductivity14,15,28,29, topological materials9,13,30,31, 1D and 2D conductivity3,10,11,28, quantum Hall efect10,32, electronic and quantum phase transitions3,12,23,33, and many other physical efects. In many of these applications one of the broadest interests is dealing with samples of irregular shapes and small sizes

Grain boundaries:

- Interface between two grains, or crystallites. 2D defects in the crystal structure, and tend to decrease the electrical and thermal conductivity