

Friedrich Schiller Universität Jena
PAF

Dissertation

High-Fluence Ion Beam Irradiation of Semiconductor Nanowires

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Abstract

Hier alles Bla

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1 Introduction

2 Sputtering of Nanowires

This chapter will investigate the sputtering of nanowires. The experiments were conducted together with Stefan Noack and are partially published in his master thesis [Noa14] and in Nano Letters [].

2.1 First results in *Mn* irradiated *GaAs*

Introduction by Mn in GaAs (JPhysD)

2.2 Simulation results

A good understanding of the sputtering of nanowires can be gained by looking at MC simulations results performed with *iradina*. From the discussion of the Sigmund sputter model in chapter ?? a maximum is expected for a certain ion, ion energy and nanowire diameter combination. This is confirmed by MC simulations shown in figure 2.1a 2.1b for the examples of Xe^+ and Ar^+ ions, respectively, irradiating a nanowire at an angle of 45° to the nanowire. Note that the color profile is not identical as sputtering is about a factor of $2,5\times$ larger for the denser collision cascades in Xe .

For both irradiations a black line indicates the ion range calculated with SRIM and projected on to 45° . The maximum of the sputtering correlates very well with the ion range. This can also be seen in 2.1c,

2.2 Simulation results

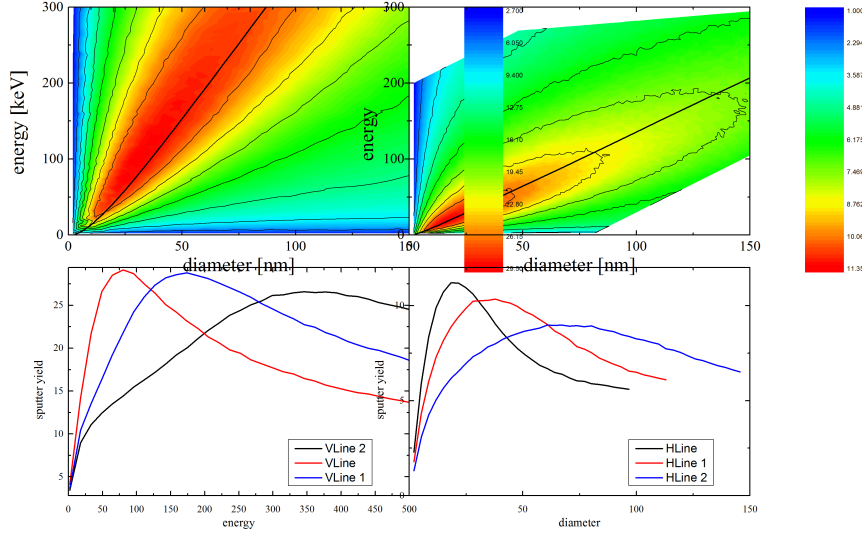


Figure 2.1: a)

where the sputter yield versus energy plot is extracted from the Xe^+ irradiation for a fixed diameter. The red, blue and black curves correspond to the irradiation of 25, 50 and 100 nm diameter wires, respectively. The maximum clearly shifts to larger ion energies for larger diameters and is found near the indicated ion range simulated by SRIM. The magenta curve shows the energy dependent sputter yield for a flat Si surface irradiated with Xe^+ ions at 45° , and simulated with identical parameters in *iradina*. The global maximum sputter yield is found at ≈ 100 keV and 30 nm. - *surface maximum*

For Sigmund sputtering model with its Gaussian ellipsoid approximation of the damage profile, a Gaussian peak is fitted to the recoil profile simulated with SRIM for both ions in Si [BZH12]. The so found mean damage depth is constantly around $0,7\times$ as less than ion range for the whole energy range investigated here. A naive first approximation with the Sigmund sputtering model would predict that the sputtering is maximal where the depth of the damage and the radius of the irradiated

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nanowire coincide. However, this is only true for central impacts, while the simulated situation is an average over all impact parameters. For non-central impacts there is less of the nanowire ‘in front’ of the ion’s path. Therefore, the maximum of the sputter yield is also at lower energies, than it would be for solely central impacts. That ion range is an even better predictor for maximum sputtering than the Gaussian fit to the damage distribution is thus a coincidental consequence of the irradiation geometry. To test the limits of the Sigmund model, a more thorough investigation of the Sigmund model’s predictions for various irradiation scenarios may be interesting, however, since the MD simulations reproduce the reality more realistically anyhow, it will not be undertaken here.

2.3 *Si* nanowire sputtering by Ar^+ irradiation

The experimental verification of the diameter dependent maximum in sputtering was investigated on etched *Si*-nanowire arrays. Figure ??a shows the principle irradiation setup illustrated by a SEM image of a single nanowire before and after the irradiation with $300\text{ keV } Ar^+$. The etched nanowire samples and the RHT allowed the simultaneous, rotated irradiation of many upstanding nanowires at $300^\circ C$. Figure ??b shows the extracted and aligned diameter versus height profile for the nanowire in figure ??a. More than 100 such profiles were semi-automatically extracted for many different nanowire diameters. The sputter yield calculated from these extracted profiles is plotted versus the local diameter in ??c for 100 and $300\text{ keV } Ar^+$.

The nanowires were irradiated rotated at an angle of 45° to the ion beam of Ar^+ at 100 and 300 keV .

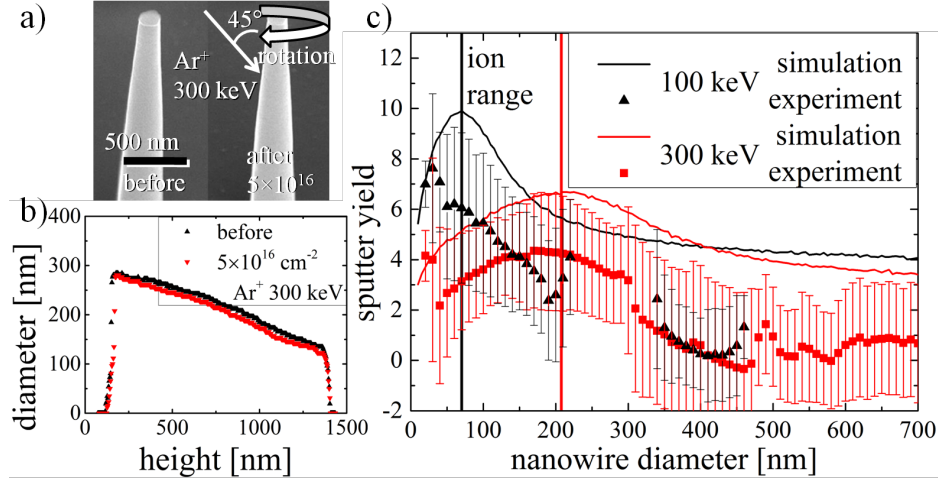


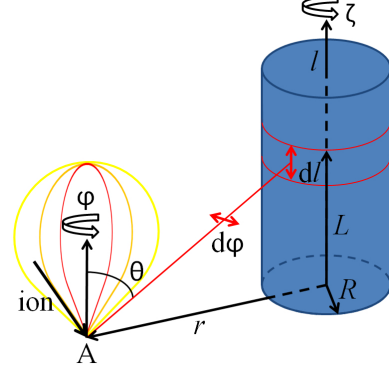
Figure 2.2: a) Exemplary SEM images of a *Si* nanowire before and after the rotated irradiation with 300 keV Ar^+ at 300°C . The extracted diameter vs. height profile for this nanowire is shown in b). From many such profiles the sputter yield vs. diameter was calculated and plotted in c) as black triangles and red squares for the irradiation with 100 and 300 keV Ar^+ , respectively. The sputter yield calculated with *iradina* simulations is shown for either case as a line-plot. The corresponding SRIM ion range at 45° is marked by a vertical line.

2.4 Redeposition

While irradiating a nanowire which is standing perpendicular on a substrate as shown in ?? material will also be sputtered from the substrate. Some of the sputtered material from the substrate will be redeposited on the nanowire, so that the observable sputter yield will be lower than the actual sputtering. Consider the situation shown in figure 2.3. An ion hits the substrate at point A. A possible path of a sputtered atom is indicated by the red line to a point on the nanowire, redepositing the substrate atom on the nanowire.

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Figure 2.3: Illustration of the redeposition of sputtered material from the substrate point A onto the nanowire with radius R at a height L . Since the wire is rotated around its axis ζ and the whole substrate is irradiated, a rotationally symmetric angle distribution for the sputtered atoms can be chosen.



The following calculation will estimate how many atoms are deposited on the nanowire, by first calculating the probability of a sputtered atom to hit it P :

$$P = \int_0^{2\pi} \int_0^{\pi/2} H(\theta, \varphi, r, R, L) \tilde{S}Y(\theta, \varphi) \cos(\theta) d\theta d\varphi. \quad (2.1)$$

Where $H(\theta, \varphi, r, R, L)$ is the probability distribution of hitting the nanowire. It is $1/(4\pi)$ if the trajectory along θ and φ from r hits the nanowire with length L and radius R , and zero otherwise. For irradiation at an angle, the angle distribution of the sputter yield $\tilde{S}Y(\theta, \varphi)$ is expected to have a preferential direction along the ion beam [VWMS08]. However, the effective distribution becomes rotationally symmetric (independent of the angle φ) if one neglects the shadowing of the ion beam on the substrate. Then all points around the wire are hit and the wire is rotated around its axis (angle ζ). This means that a rotationally symmetric angle distribution $\tilde{S}Y(\theta)$ of the sputtered atoms from the substrate can be used, as indicated by the yellow, orange and red bulbs in figure 2.3. A $\cos^\kappa(\theta)$ distribution is chosen, as it forms flattened angle distributions for $\kappa < 1$, which can emulate the rotation of a slanted angle distribution:

2.4 Redeposition

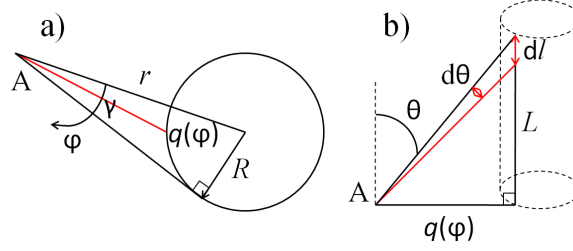


Figure 2.4: a) On the substrate surface R is the radius of the nanowire, r the distance from the point of impact A to the center of the wire, $q(\phi)$ the distance to the wires surface at the base of the wire. The angle between r and the tangent to the nanowire circumference is γ . b) Side on view with θ the angle to the substrate normal of the trajectory to hit the wire at L .

$$\tilde{S}Y(\theta) = \frac{SY \cdot \cos^\kappa(\theta)}{\int_0^{2\pi} d\tilde{\varphi} \int_0^{\pi/2} \cos^\kappa(\tilde{\theta}) \cos(\tilde{\theta}) d\tilde{\theta}} = SY/c(\kappa) \cdot \cos^\kappa(\theta), \quad (2.2)$$

where the denominator $c(\kappa)$ normalizes the angle distribution function $\cos^\kappa(\theta)$ and SY is the total sputter yield from the surface. The parametrization of $H(\theta, \varphi, r, R, L)$ in φ is straightforward, as the integration bounds for φ are $[-\gamma, \gamma]$ with $\gamma = \arcsin(R/r)$ the angle between r and the tangent to the nanowire in figure 2.4a. To solve the integration over θ it is useful to express the distance q from the impact point to the base of the nanowire as a function of $\rho = R/r, r$ and φ :

$$q(\rho, r, \varphi) = r \cdot \sqrt{1 + \rho^2 - 2\sin^2(\varphi) - \sqrt{\cos^2(\varphi)(\cos(2\varphi) - 1 + 2\rho^2)}}. \quad (2.3)$$

Then the integration over θ can be substituted by an integration over the length of the nanowire l . The substitution can be found looking at figure 2.4b:

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$$\begin{aligned} d\theta &= \frac{\sin(\theta)}{\sqrt{L^2 + q^2}} dL \\ \theta &= \arctan(q/L) \end{aligned}$$

Inserting into equation 2.1 and simplifying yields:

$$P = \frac{2 SY}{c} \int_0^\gamma \int_{L_1}^{L_2} \frac{l^{\kappa+1} q}{(l^2 + q^2)^{(\kappa+3)/2}} dl d\varphi. \quad (2.4)$$

With $l^* = L_1 - L_2$ the area hit on the nanowire is now $\pi R l^*$, positioned at the height $L = (L_1 + L_2)/2$ as indicated between the two red lines in figure 2.3. Integrating the probability P to hit the nanowire at each substrate position over the whole substrate area and normalizing it to the area of the nanowire which is hit yields the number of atoms N hitting the nanowire per fluence Φ :

$$N/\Phi = \frac{2 SY}{c\pi R l^*} \int_0^{2\pi} d\zeta \int_R^\infty \int_0^\gamma \int_{L_1}^{L_2} r \frac{l^{\kappa+1} q}{(l^2 + q^2)^{(\kappa+3)/2}} dl d\varphi dr. \quad (2.5)$$

The integration can be solved numerically using the numerical integration tools CQUAD and QAGI [Gou09]. Perhaps counter-intuitively, the result is independent of the nanowire radius R and the height at L at which the deposition is calculated. The redeposition amounts to $10\% \cdot \Phi \cdot SY$ for the very broad distribution when $\kappa = 0.25$. As already shown in figure 2.1c, the sputter yield (SY) is significantly lower on the plane substrate than on the nanowire to begin with. Therefore, the redeposition can be safely neglected for the evaluation of sputtering. As the atoms sputtered from the substrate have a very low energy, they will be deposited on the surface of the nanowire. This makes them prone to re-sputtering, which reduces the finally incorporated number of sub-

2.5 *Discussion*

strate atoms even further. Nevertheless, care is advised in the choice of the substrate material, as the incorporation of substrate atoms in the nanowire may have detrimental doping effects.

2.5 Discussion

3 Summary and Outlook

check: Master Thesis Noack, Ogrisek, Conference proceeding D. Sage, Rutherford, Nordlund

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