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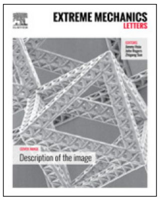

Erosive-thermal transition in high-flux focused ion beam nanomachining of surfaces

K. Das [a], J.B. Freund [a,b], H.T. Johnson [a,*]

[a] *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, 1206 W. Green St., Urbana, IL 61801, United States*

[b] *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign, 104 S. Wright St., Urbana, IL 61801, United States*

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ABSTRACT

Focused ion beams (FIB) are increasingly used for surface modification and fabrication with nanometer scale precision. In FIB, an energetic beam of ions strikes a surface and removes material, a process that is understood to depend upon the properties of the beam (e.g. beam flux, ion energy) and is thought to be due to ion induced sputter erosion. We show that the material removal rate is also strongly affected by the thermal properties of the material, sample temperature, and geometry. Furthermore, we deduce a dimensionless parameter, a ratio of incident power to thermally dissipated power (Q_{FIB}), which parameterizes a switch of the underlying mechanism of material removal. It predicts with remarkable accuracy a previously overlooked transition from slow erosive material removal to significantly accelerated thermal vaporization material removal. Its critical value explains an observed transition in data covering a range of beam fluxes, ion energies, spot sizes, film thicknesses, materials, ion species, and temperatures. Large-scale parallel molecular dynamics simulations support this transition.

Ion beam flux, defined as the number of ions incident on a surface per unit area per unit time, is a fundamental parameter in FIB material processing. A corresponding beam current is easily computed from the flux, since each incident ion typically brings one charge to the surface, though electrostatic or charge neutralization effects might alter any direct correspondence. Thus, with the beam flux (or the current) and the nominal sputter yield (the number of sputtered atoms per incident ion, typically near 1) it is simple to estimate a material removal rate during FIB processing. For example, for a widely studied material like silicon, with typical ion energies (30–50 keV) and currents estimated from reported beam spot size (typically < 1 pA), the expected sputter yield (SY ≈ 2.0) [1] yields the independently measured erosion rates in Table 1 [2–5].

However, several recent studies report material removal rates that are orders of magnitude higher than such estimates. Table 1 presents results for a variety of conditions: energies from 15 to 200 keV; beam currents ranging over three orders of magnitude; target materials including metals, semiconductors, and polymers; various dwell times, pixel sizes, and ion beam species. In many cases, the corresponding estimate of number of incident ions required to remove the observed volume of atoms is a factor of $\sim 10^3$ larger than the actual number of ions delivered. We describe this phenomenon with a parameter called normalized material removal rate (R_{MR}) representing the ratio of the observed volume of material removal to the expected volume of material removal based on a sputtering mechanism.

Various explanations have been proposed for these anomalous results. Matovic et al. [6] suggest that the high sputter yield they deduce is due to the small thickness of the film, which renders the system inefficient in

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[*] Corresponding author.
E-mail address: htj@illinois.edu (H.T. Johnson).

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Table 1
Normalized material removal rate (R_{MR}) for previously reported FIB experiments.

Material	(D, L) or (W, H) (nm, nm) $V_{\text{milled}} = \pi D^2 L/4$, $V_{\text{milled}} = W^2 H$	Nominal current (pA) I	Beam energy (keV) E	Dwell time, number of passes t	Ions delivered $N_d = \frac{It}{e}$	Atoms removed $N_a = \frac{V_{\text{milled}}}{V_{\text{atom}}}$	Ions required $N_r = \frac{N_a}{SY}$	Normalized material removal rate $R_{MR} = \frac{N_r}{N_d}$
(Cr/Si/O) [6]	50, 10	5	30	0.02 ms, 4	2.5×10^3	15×10^6	7×10^6	2.8×10^3
PMMA [7]	1700, 300	150×10^3	15 (electron)	10 µs, 1	9.36×10^6	3.4×10^{10}	1.7×10^{10}	1.8×10^3
Si [2]	1000, 150	1.5	30	580 µs, 1	355×10^6	7.5×10^9	3.75×10^9	10.6
Si [3]	300, 300	48	30	0.1 ms, 12	431×10^6	1.06×10^9	530×10^6	1.23
Si [4]	20, 20	11	30	100 µs, 1	6.86×10^3	314×10^3	157×10^3	22.9
Si [5]	10 000, 40	150	30	1 µs, 1	5×10^{10}	1.99×10^{11}	1×10^{11}	2
Au [8]	10, 50	–	200 (Xe)	–	1	20×10^3	10×10^3	10×10^3
PMMA [9]	60, 5	1	30	20 µs, 1	MRR $= 1000\ \mu\text{m}^3/\text{nC}^9$		MRR $= 1\ \mu\text{m}^3/\text{nC}^{10}$	1×10^3

dissipating heat from the impact zone. As a result, the temperature within the zone is expected to significantly exceed the melting point. For sufficiently high flux, they claim that a hole is created via evaporation.

Liu et al. [9] report FIB material removal that is more than 10^3 faster than that predicted by sputter yield for PMMA membranes. They speculate that the anomalous sputter yield, of 10^4 atoms/ion by their own estimate, is due to an ion-enhanced degradation mechanism, an unzipping reaction which, without ion beam irradiation, would only be observed at high temperatures.

Kolíbal et al., [2] Hopman et al., [3] and Li et al. [4] study the dependence of enhanced material removal rate of Si on dwell time (1 µs–5 ms) and beam energy (5–30 keV). They observe increased material removal rate and report that the discrepancy depends on the beam parameters, namely increased dwell time and ion beam energy.

Particularly relevant to the present results, Chu et al. [7,10] measure the temperature rise in a 300 nm thick, 40 µm wide PMMA substrate, due to two experiments with a 15 kV electron beam: one with FWHM 1.7 µm and 150 nA and the other with 2.0 µm and 600 nA. They report an 18 K temperature increase of the substrate after 100 µs. If we consider the electron beam or ion beam as a localized thermal source, and for simplicity assume constant bulk thermal properties of the material, our continuum finite element simulation [11] suggests that such a temperature increase corresponds to a local target temperature of nearly 9000 K at the center of the beam over a 400 nm spot. While obviously unphysical, this does suggest that an extreme thermal effect may be responsible for the anomalous material removal rate.

Similar temperature distributions are calculated by Schmied et al., [12] who model spatial temperature evolution in HDPE (high density polyethylene), PMMA, and silicon due to FIB processing. They use SRIM to estimate ion energy deposition and energy dissipation to phonons, along with calculations based on a thermal spike model [13]. Using this model, they simulate a 30 keV Ga ion beam with 40 nm FWHM and 500 pA beam current, parameters readily achieved using commercial FIB instruments. In this case they find a peak temperature of 6300 K for PMMA, 2400 K for HDPE, and 400 K for Si. They also perform FIB experiments with a 30 keV Ga ion beam, with 40 nm FWHM at 500 pA and 500 µs dwell time in PMMA and HDPE materials. The material volume removed by the FIB process in the milled structures matches well with their thermal system predictions.

Orthacker et al. report similar FIB experiments in a range of soft materials [14]. They observe an enhanced material removal rate (factor of $\sim 10^3$) when the dwell time is increased or when the distance between two neighboring target pixels is decreased. Although observed material removal rates in silicon tend to be much lower than in soft materials, increased dwell time also enhances the rates in silicon [2,3]. Indeed, increasing dwell time or decreasing point pitch increases the temperature near the ion beam impact zone significantly, leading to volatizing effects as reported by Orthacker et al. [14] This evidence points to the possibility that the accelerated material removal may be due to a thermal loading condition.

Molecular dynamics simulations of FIB bombardment of silicon provide a microscopic model of FIB mechanisms. Our results, summarized below, show in detail that for increasing beam flux, material removal suddenly changes from a sputter erosion driven process at lower fluxes to a thermally driven process at higher fluxes [15].

Together, these studies suggest an orders-of-magnitude variability in material removal rates depending on the beam current, beam energy, material properties, and other parameters. Low thermal conductivity materials are more susceptible to large temperature increases. Similarly, enhanced material removal is often observed in thin membranes, and for longer beam dwell times and denser target pixel distributions.

Target properties and the specifics of the FIB instrument, shown schematically in Fig. 1, both affect material removal. Parameters include ion beam energy (E, typically measured in keV), time between impacts (δt, in picoseconds), ion beam current (I, in Amperes), accelerating potential (V, in Volts), ion beam flux (ϕ, ions/m^2/s), target material thermal conductivity (k, Wm^{-1} K^{-1}), target layer thickness (h, in nanometers), penetration depth (p, in nanometers), FWHM diameter of the beam (d, in nanometers), and a characteristic temperature difference (ΔT, in Kelvins). Here we define $\Delta T = T_b - T_s$, where T_b is the boiling temperature of the material, and T_s is the target temperature. Using these we construct a dimensionless number to anticipate a thermal threshold behavior in the material removal rate.

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