

Roughening Mechanisms for Heated Surfaces

Executive Summary

The roughening of surfaces by ions, x-rays, and lasers has been studied for decades. In many cases, there is still dispute regarding the mechanisms for this phenomenon. This controversy likely is caused by the existence of many roughening mechanisms, depending on the irradiation parameters and the material being irradiated. In my opinion, the likely mechanism for roughening of samples in RHEPP and on the Z-machine is thermomechanical in nature. In metals, it is likely a result of the ratcheting of cyclic plastic strain resulting from surface thermal stresses. In ceramics, it is likely the result of brittle fracture due to cyclic thermal stress. In either case, the roughening can be minimized by using longer pulses or lower fluences.

Introduction

There are numerous mechanisms for the roughening of heated surfaces. This brief paper discusses surface effects due to melting, thermomechanical behavior, and oxidation. Theoretical predictions are provided for the fluence required to melt or sublimate, and yield or fracture a material.

Phase Change

An obvious mechanism affecting heated surfaces occurs when the heating is sufficient to melt the target material. The resulting surfaces in this case often exhibit periodicity resulting from either resonant periodic structures (RPS), or non-resonant periodic structures (NRPS). RPS result from an interaction between the incident radiation and electromagnetic waves that propagate across the surface and can be created either from a single pulse or multiple pulses. The character of the structure is generally determined by the wavelength, polarization, and incident angle of the radiation. The mechanism involves a modulation of the absorbed surface energy, resulting from an interaction between the incident radiation and surface electromagnetic waves.

In the case of NRPS the structures do not result from electromagnetic interactions, but from material behaviors. Formation of an NRPS generally requires multiple pulses, with increasing order as the number of pulses increases. The period of such structures is generally found in the range of 1-50 microns, depending on the intensity of the radiation, the target material, and the number of pulses. Melting is required in each pulse and formation of an NRPS is always accompanied by erosion. The mechanisms for formation are not clear at this point, but many believe that the structures result from non-uniform vaporization of the surface resulting from instabilities at the interaction face.

To estimate the heating that will just cause melting, one can assume uniform heating on a semi-infinite body. These assumptions are valid as long as the diffusion length is short compared to the thickness of the sample and to the characteristic dimension of the heated spot size. The diffusion length must also be long relative to the deposition length of the incident radiation. For the purposes of this discussion, the diffusion length can be taken to be

$$\eta = \sqrt{\kappa t_p}$$

where η is the diffusion length, κ is the thermal diffusivity, and t_p is the pulse length. Under these assumptions, melting will just occur when

$$q_m = \frac{T_m k \sqrt{\pi}}{2 \eta}$$

where q_m is the absorbed heat flux that will just melt the surface, T_m is the melt temperature, and k is the thermal conductivity. In many cases only the fluence deposited during the pulse is known. If we refer to the energy fluence necessary to just melt the surface as

$$\Gamma_m = q_m t_p$$

then we find

$$\Gamma_m = \frac{T_m k}{2} \sqrt{\frac{\pi t_p}{\kappa}}$$

This result assumes that the heating is a step function in time. Values for the fluence to melt a surface are given in the following table for several materials and pulse lengths.

Material	Thermal Conductivity W/mK	Density kg/m ³	Heat Capacity J/kgK	Melting or Sublimation Temperature K	Fluence*	Fluence*
					to Just Melt Surface (10 ns pulse) J/cm ²	to Just Melt Surface (20 ns pulse) J/cm ²
Rhenium	48	21020	130	3459	0.35	0.50
SiC	40	3210	580	3100	0.24	0.34
Tungsten	170	19250	130	3695	0.68	0.96
Nickel	91	8908	444	1728	0.29	0.41
Aluminum	235	2700	897	933	0.20	0.28
Graphite	140	1860	711	3923	0.47	0.67
Copper	400	8920	385	1358	0.45	0.63

*Note that this fluence assumes no reflectivity so it is equivalent to absorbed fluence.

Plastic Deformation in Metals

In order to avoid roughening of a surface by incident radiation, one must first avoid melting. Given this, one can still induce permanent deformation by forcing yielding of the target. For short pulses, one can generally assume that the peak surface stress is zero perpendicular to the surface and the resulting transverse stress is then given by

$$\sigma = \frac{E \alpha T}{(1 - \nu)}$$

where E is the elastic modulus, α is the thermal expansion coefficient and ν is Poisson's ratio. Hence, yielding in a metal will occur when this stress reaches the yield stress (Y), giving the fluence sufficient to yield the surface as

$$\Gamma_Y = \frac{Y(1-\nu)k}{2E\alpha} \sqrt{\frac{\pi t_p}{\kappa}}$$

Values of this parameter are given in the table below for various materials and pulse lengths.

Material	Elastic Modulus GPa	Poisson's Ratio	Thermal Expansion Coefficient /K	Yield or Fracture Strength* MPa	Fluence to Just Yield Surface (10 ns pulse) J/cm ²	Fluence to Just Yield Surface (20 ns pulse) J/cm ²
rhenum	463	0.3	6.20E-06	290	0.007	0.010
SiC	466	0.21	4.00E-06	595	0.019	0.027
tungsten	411	0.28	4.50E-06	1506	0.107	0.152
nickel	200	0.31	1.34E-05	420	0.018	0.026
aluminum	70	0.35	2.31E-05	33	0.003	0.004
graphite	12	0.2	6.00E-06	65	0.087	0.123
copper	130	0.34	1.65E-05	262	0.026	0.037

*Note that the strength will depend dramatically on the preparation of the material, so the numbers in the table above are meant to be merely suggestive of the expected behavior. In the cases of SiC and graphite, fracture, rather than yielding, is the failure mode.

As expected, the fluence to cause yielding is significantly below that to cause melting. Hence, for the fluences usually seen in the RHEPP and Z experiments, yielding or fracture is expected and this is thus a likely cause of the surface roughening.

The mechanical behavior in cases where multiple pulses are incident on a surface can be quite complex. If the energy density is not sufficient to yield the surface, one can still produce fatigue cracks due to the cyclic stress. If yielding does occur, but the stress is just above the yield stress, then one would expect plastic deformation on the first cycle, but elastic behavior thereafter. On the other hand, when the stress calculated using elastic theory is twice the yield stress, then one would expect plastic deformation on each cycle and an accumulation of plastic strain leading to cavitation and fracture. In this case, the deformation tends to occur along closely spaced slip planes (slip bands), which expand and form intrusion and extrusion steps at the surface. The spacing of these steps is thought to depend on the mean free path for vacancy motion.

Brittle Materials

Brittle materials do not yield like metals. They fail due to catastrophic fracture as a flaw rapidly propagates through a solid. This process is complex, but can be approximated by the use of the thermal stress formulas given in the previous section and

a uniaxial fracture stress. Detailed fracture mechanics analyses are necessary to provide detailed predictions regarding surface roughening in these materials, but this is beyond the scope of this summary. Results were provided for SiC and graphite in the previous section.

Ion Damage

In the case of ion-induced damage, displacement phenomena can cause surface damage. This sputtering can create a variety of surface features, including cones and ripples, in both metals and ceramics. The characteristic dimensions of these features are typically on the order of 0.1 to 10 microns. Most studies employ ions with energies less than about 10 keV to fluences below 10^{18} ions/cm². Several theories exist for the parameters that determine the size of these features.

Laser-Induced Oxidation

A final mechanism for surface roughening is laser-induced oxidation. When a material is heated in an oxidizing environment, small oxide crystals can form, altering both the optical and thermomechanical characteristics of the surface. These crystals are typically much less than one micron in size and can lead to surface roughening.

Conclusions

The damage induced in RHEPP and the Z-Machine is likely due to thermomechanical phenomena. In metals, the accumulation of plastic strain due to cyclic thermal strain is the likely cause, primarily in the form of localized slip bands. In brittle materials, the likely cause is local brittle fracture in the neighborhood of existing flaws or inclusions. Other possible mechanisms include sputtering due to ion bombardment and laser induced oxidation. If thermomechanical effects are indeed the cause, they can be alleviated by using longer pulse times and/or lower fluences.

Bibliography

E. Eklund, et al, "Submicron-Scale Surface Roughening Induced by Ion Bombardment," *Phys. Rev. Lett.*, **67 (13)**, 1991, 1759.

H. Musal, "Thermomechanical Stress Degradation of Metal Mirror Surfaces Under Pulsed Irradiation," *Laser Induced Damage in Optical Materials*, 1979, National Bureau of Standards, **568**, 1980, p. 159.

A. M. Prokhorov et al, **Laser Heating of Metals**, Adam Hilger, Bristol, 1990.

G. Wehner, "Cone Formation as a Result of Whisker Growth on Ion Bombarded Metal Surfaces," *J. Vac. Sci. A*, **3 (4)**, 1985, 1821.