DOE Final Report

Mechanisms of sputter ripple formation: coupling among energetic ions, surface kinetics, stress and composition

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Overview of technical accomplishments over entire project

Self-organized pattern formation enables the creation of nanoscale surface structures over large areas based on fundamental physical processes rather than an applied template. Low energy ion bombardment is one such method that induces the spontaneous formation of a wide variety of interesting morphological features (e.g., sputter ripples and/or quantum dots). This program focused on the processes controlling sputter ripple formation and the kinetics controlling the evolution of surfaces and nanostructures in high flux environments. This was done by using systematic, quantitative experiments to measure ripple formation under a variety of processing conditions coupled with modeling to interpret the results.

An example of ripple formation on a Si surface is shown in figure 1. The graph (figure 1a) shows the ripple wavelength vs time for several different fluxes. The AFM images beneath it (figure 1b) show the evolving surface morphology with increasing time (fluence). For this flux, the wavelength is found to be constant with time, consistent with an instability mechanism for ripple formation.

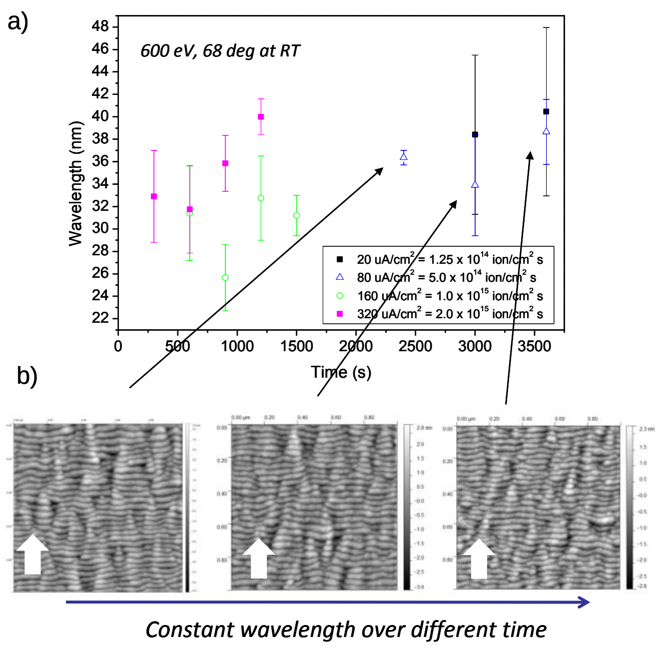

Figure 1. a) Ripple wavelength vs time for several fluxes. B) Surface morphology showing constant wavelength with time.

Studies such as these established a quantitative foundation for ripple formation, allowing the development of a kinetic phase diagram that showed how different regimes of pattern formation depend on the temperature and flux. Continuum models and Kinetic Monte Carlo (KMC) simulations were used to show that the atomistic mechanisms included in the models lead to the type of patterning behavior observed.

However, these experiments also illustrated serious discrepancies between the model and the experiments, i.e., the rate of ripple growth seen experimentally was much slower than predicted by the model (e.g., a factor of >100 for our measurements of Cu). We therefore focused in the final stages of the project on considering other mechanisms that might account for the enhanced growth rate of ripples. Note that this level of understanding could not have been achieved without the systematic experiments and modeling that related ripple formation to the processing conditions.

Summary of impact

The following report summarizes the significant contributions that our DOE-funded program has made to understanding the fundamental mechanisms of ripple formation. The program has resulted in 32 publications (including invited reviews in Journal of Applied Physics [1] (cover shown in figure 2) and J. Phys. Cond Mat [2,3] and 3 book chapters) and 45 presentations (18 invited to international meetings). Our Phys. Rev. Lett. in June 2007 on composition modulations during sputtering was highlighted in the table of contents as an editor's suggestion, chosen "to promote readings across fields". A list of the publications and presentations is given in the section following the results of the research program.

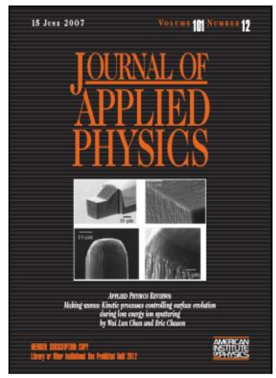

Figure 2. Invited review published in J. Appl. Phys. 2007.

Summary of research results

<u>Quantification of BH ripples and linear instability in Cu</u>

The early work in this program was focused on the systematic study of ripple formation kinetics within the context of the Bradley-Harper (BH) linear instability theory. The measurements were performed on Cu surfaces because, prior to this work, BH-type ripples had only been observed in semiconductors and insulator materials. Measurements of ion-induced pattern formation on metal surfaces had been of the type controlled by Ehrlich-Schwoebel (ES) barriers to surface diffusion. Our results showed that in the appropriate kinetic regime (higher flux and temperature than previous studies), ripples of the BH-type could in fact be formed on the Cu surface [4]. The ripples were oriented with the ion beam direction, had a fixed wavelength and grew exponentially in the early stage.

Measurements of the wavelength as a function of flux and temperature (figure 3) [5] showed a complex non-Arrhenius behavior and a flux dependence that is different at high T ($\lambda \sim f^{1/2}$) and low T ($\lambda \sim f^{0}$). These results could be understood within the context of the BH model by considering the dependence of the defect concentration on the flux and

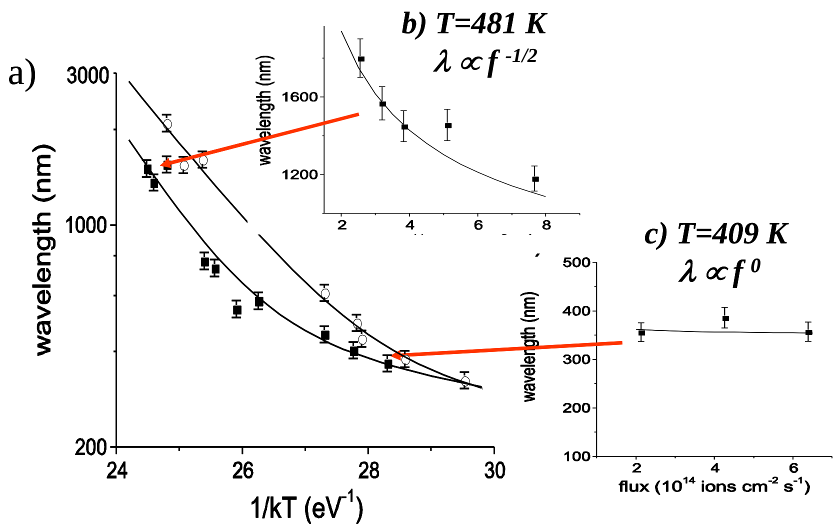

Figure 3. Measurements of the ripple wavelength on Cu(001) as a function of a) temperature and as a function of flux at b) T = 481K and c) T= 409 K. The solid lines are a fit to a model based on the BH theory with a temperature- and flux-dependent defect concentration.

temperature. Chan et al. [1] developed a model for the surface defect concentration that included thermal and ion-induced defect generation processes:

$$C_{ave}(f,T) = n_0 \exp(-E_f / kT) + \frac{4l^2}{3D_0} Yf \exp(E_m / kT) \qquad (1)$$

where Y refers to the sputter yield. At low temperature the defects are primarily created by the ion beam while at high temperature the defects are formed thermally so that the average concentration is dependent on the temperature and flux. The combination of the BH theory with this defect model explains both the temperature and flux dependence of the wavelength (solid lines in figure 3).

<u>Kinetic Monte Carlo (KMC) simulations</u>

In addition to the experimental studies of BH ripples, we developed a KMC simulation model that included the Sigmund mechanisms for sputtering as well as diffusion of ion-induced vacancy and adatom defects [6]. In the KMC simulations, the interaction between the ion and surface is identical to the one in the Sigmund model, in contrast with the experiments in which we cannot be sure of the ion-solid interaction. The defect kinetics are implemented by allowing the individual atoms to hop around with transition rates that depend on the local atomic configuration which allows the actual time dependence of the surface evolution to be simulated. In addition, we allow the vacancies on the surface to be mobile, consistent with measurements of surface vacancy diffusion on Cu that indicate the vacancies are mobile. The presence of mobile vacancies is essential to the ripple formation since there are more vacancies created during ion bombardment than adatom-type defects. In comparing the KMC with the BH theory, we do not need to model the defect concentration but can instead count the actual number of defects on the surface.

An image of the simulated surface morphology and results for the simulated wavelength at different temperatures and fluxes is shown in figure 4. We find that the temperature and flux dependence of the wavelength and growth rate can be well explained by the BH theory (solid lines in the figure). This result validated that the BH model is a good continuum approximation for the surface evolution when the ion-solid interaction is modeled by the Sigmund mechanism. In particular, the relationship between the ripple growth rate and the ripple wavevector is explained well by the BH theory. This is in marked contrast with the experimental studies in which the measured ripple growth rate on Cu is significantly faster than the growth rate predicted form the BH theory using reasonable approximations for the ion parameters in the Sigmund mechanism. This is a strong indication that there may be other mechanisms in the actual experiments beyond those included in the BH model. In addition to the growth rate, the KMC simulations also predict that the ripples travel with a velocity across the surface. The simulated velocity also agrees well with the prediction of the BH theory, including the wavelength dependence of the velocity (dispersion). This is significant because recent experiments [7,8] have found that the ripples on amorphous surfaces produced by focused ion beams travel in the opposite direction predicted by the theory. The simulations however indicate that the predicted BH velocity is consistent with what occurs for sputtering based on the Sigmund model.

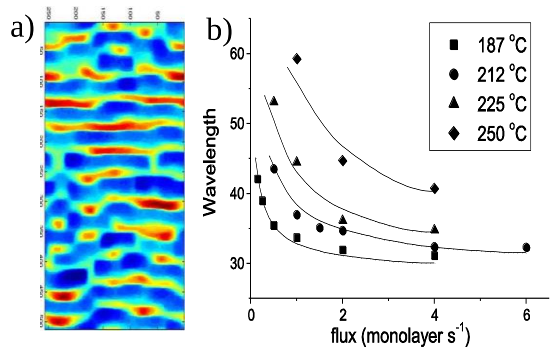

Figure 4. a) Simulated ripple morphology and b) simulated ripple wavelength as a function of flux and temperature. Solid lines are fits to BH theory using simulation parameters.

Kinetic regimes of ion patterning

In a review for J. Appl. Phys. [1], we presented a comprehensive picture of ion-induced patterning in terms of the different atomistic mechanisms that had been proposed and the kinetic regimes in which they operate. We showed how a wide range of behavior observed on Cu surfaces could be organized in terms of a “kinetic phase diagram” (figure 5) that delineated the different regimes of temperature and flux in which they were observed (BH ripples, Ehrlich-Schwoebel or diffusion controlled patterns, athermal ripple

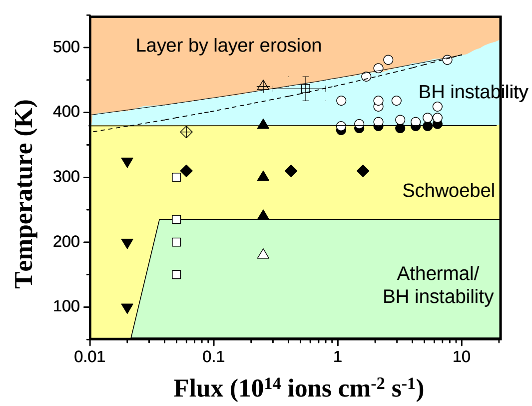

Figure 5. Kinetic phase diagram shows regimes of pattern formation observed on Cu(001) surfaces at different fluxes and temperatures.

formation, non roughening behavior). The relationship between the different regimes can be understood in terms of the linear instability model using the different kinetic mechanisms described earlier. The wavevector-dependent growth rate for all these processes acting together is given by:

$$r(k_x,k_y) = -\nu_x(f)k_x^{\,2} - \nu_y(f)k_y^{\,2} + S_x(f,T)k_x^{\,2} + S_y(f,T)k_y^{\,2} \\ - B(f,T)k^4 - B_{I,x}(f)k_x^4 - B_{I,xy}(f)k_x^2k_y^2 - B_{I,y}(f)k_y^4 \qquad (2)$$

where the parameter *S* comes from the instability due to the ES barrier [9]. The different pattering behavior arises because the parameters can have different dependence on the processing conditions of *f* and *T* so that different processes will dominate in different kinetic regimes. For instance, the roughening due to ES barriers is maximum at intermediate temperatures so that a transition from ES behavior to BH ripples can be observed by raising the temperature. Similarly, lowering the ion flux can induce a transition from BH ripple formation to non-roughening behavior.

Comparison of different observations with the linear instability model also served to highlight the shortcomings of the BH theory and identify where other mechanisms or effects must be considered [1]. For example, the quantitative predictions of the BH theory for the growth rate of the ripples is consistently lower than the measured rate (by 200X for Cu), suggesting that other mechanism may be contributing to the roughening. In addition, saturation of the ripple amplitude or formation of quantum dot-like structures at normal beam incidence are outside the limits of the linear theory.

Stress effects in ripple formation

The large difference between the measured ripple growth rate on Cu from the BH prediction suggested that there are other effects contributing to the ripple formation beyond sputtering. One potential mechanism is the effect of stress induced by the ion bombardment. In order to study this, we measured the stress induced in the near-surface region by the ion bombardment [10]. Surprisingly, there has been very little study of this ion-induced stress in the low energy regime typical of ripple formation. The stress during ion bombardment was measured using wafer curvature in real time during the bombardment (figure 6). We found that the stress was highly transient, decreasing rapidly after the beam was turned off. We modeled the ion-induced stress in terms of the balance between point defects (implanted Ar, vacancies and interstitals) created by the ion beam. Volumetric expansion or relaxation around each defect was used to relate the induced stress to the depth-dependent concentration of each defect. Numerical calculations of the defect concentration evolution (including

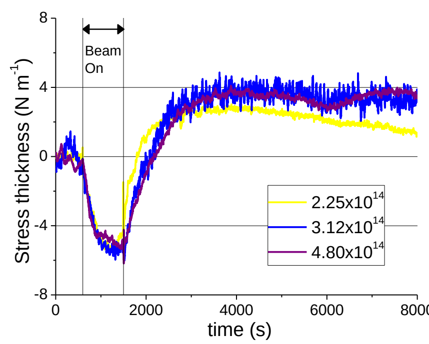

Figure 6. Measurements of stress evolution in Cu during low energy ion bombardment at different fluxes.

annihilation between the different defects) were used to understand the evolution to a steady-state stress distribution. Results of these calculations for the depth-dependent defect concentration are shown in figure 7 after different amounts of sputtering.

Surface morphology changes can relax the stress in the surface which leads to a surface instability similar to the BH mechanism (referred to as the Asaro-Tiller-Grinfeld or ATG instability). In this picture, the rate of surface roughening depends on $\partial^3 h/\partial x^3$ [11]. We combined the stress induced roughening with the BH mechanism for curvature-dependent sputter yield to develop a continuum model for the surface evolution under the combined effects of sputter removal and ion-induced stress [3]. The combination leads to a linear instability model with a rate that depends on the wavevector as $r = A|\mathbf{k}|^2 - B|\mathbf{k}|^4 + C|\mathbf{k}|^3$. The predicted wavevector and roughening rate are given by:

$$k^* = \frac{1}{2}k_{ATG} + \sqrt{\left(\frac{1}{2}k_{ATG}\right)^2 + k_{BH}{}^2} \qquad (3a)$$

$$r^* = \frac{1}{2}Ak^{*2}\,(1 + \frac{\alpha}{(4k^* - 3\alpha)}) \qquad (3b)$$

where $k_{BH} = (A/(2B))^{1/2}$, $k_{ATG} = 3\propto/4$ and $\propto = C/B$. This theory predicts that the ripple will grow faster in the presence of stress than in the simple BH theory, with a rate that rises as the wavevector approaches the value predicted by the ATG theory.

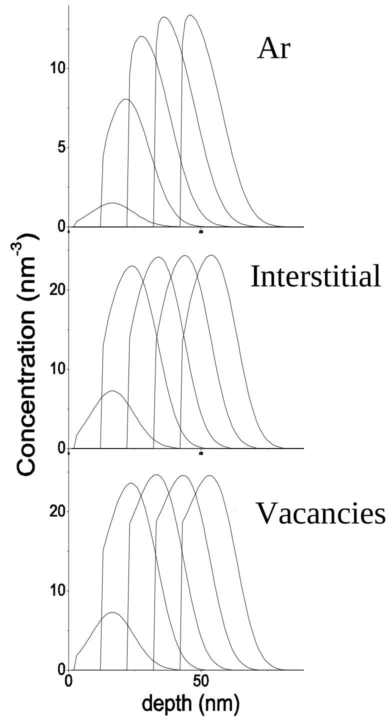

Figure 7. Results from model for defect concentration vs. depth for sputtered surfaces. Stress was calculated from concentration profiles based on relaxation volume around each defect.

<u>Prediction of composition modulations</u>

The linear instability theory described previously considers the evolution of a surface due to a balance between sputter roughening and surface diffusion in a single component system. We extended this model to consider the sputtering of alloy surfaces [12] and found that sputtering can be used to produce composition modulations on the surface, in addition to height modulations. Composition modulations arise when each component of the alloy (A, B) has a different sputter yield (Y_A, Y_B) and/or surface diffusivity (D_A, D_B). The difference in sputter yields leads to a different steady state concentration on the surface relative to the bulk. The sputter yield is taken to have the same curvature dependence for both of the components. The difference in diffusivity and yield leads to the development of a sinusoidal composition modulation.

The results of the model indicate that the surface will develop modulations in the height and also in the composition on the surface (figure 8). Depending on the relative values of the diffusivities and sputter yields, the phase between the surface height and the composition modulation can be changed. If $D_A/D_B > Y_A/Y_B$, then the composition of A will be enriched at the bottom of the ripple. For the opposite case, the composition of A will be enriched at the top of the ripple. The theory predicts that the composition modulations can be significant. The amplitude of the composition modulation (ζ) depends on the relative values of the diffusivity and yield as shown in figure 8; the maximum modulation can be as large as 0.7. Although this model predicts composition modulations, there has not yet been an experimental verification of the effect. Looking for these modulation is a part of the proposed experimental work.

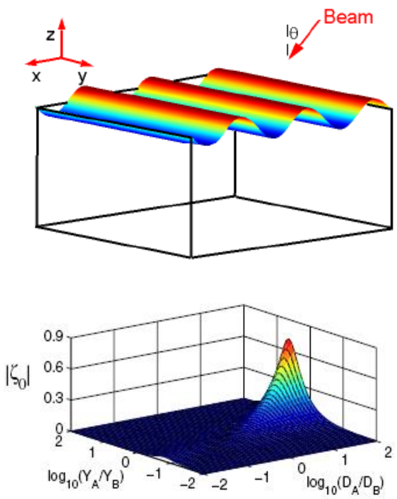

Figure 8. (Top) Schematic of composition modulations (shown by color variations) that accompany shape modulations on an alloy surface predicted by our theory. (Bottom) The amplitude of composition as a function of the ratio of the yields and diffusivities.

Relaxation of alloy surfaces

As an alloy surface evolves under capillary forces, differing mobilities of the individual components can lead to kinetic alloy decomposition at the surface (figure 9). We have addressed the relaxation of nanoscale faceted and rough sinusoidal ripples on alloy surfaces by considering the effects of both *surface* and *bulk* diffusion. On rough surfaces, in the absence of bulk diffusion, we have derived exact analytical expressions for relaxation rates and identified two natural time scales that govern the relaxation dynamics. Bulk diffusion was shown to reduce kinetic surface segregation and enhance relaxation rates, owing to intermixing near the surface. Our results provide a quantitative framework for the interpretation of relaxation experiments on alloy surfaces, which we plan to carry out as part of this renewal proposal.

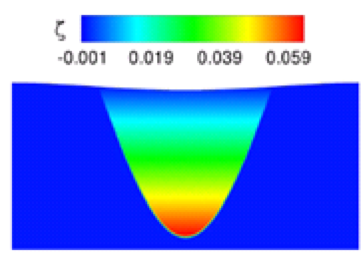

Figure 9. Vertical compositional gradients for an almost fully relaxed sinusoidal ripple modulation with D_A□$/D_B$=100. The enrichment in the *A* species at the bottom of the “valley” occurs due to rapid diffusion of fast-moving *A*

In the case of faceted alloy surfaces, we find that the interplay of material transport kinetics and singular features associated with facets leads to evolution behavior that is remarkably different from that of unfaceted or rough surfaces. In the latter case, kinetic alloy decomposition arising from the differences in the mobilities of the alloy components, progressively evolves to the equilibrium composition as the surface relaxes. In contrast, the presence of facets permanently locks the surface composition at a non-stoichiometric, near-constant profile during relaxation. Based on scaling laws derived from an analytical model, we find that small feature sizes and large differences in diffusivities can enhance composition locking on faceted surfaces.

<u>KMC simulations of ripple formation with ES barriers</u>

The continuum model predicts that the flux-normalized amplification rate of the ripple amplitude (*r*/f)* depends on the square of the ripple wavevector (*k**). As shown in figure 10, the computer simulations using KMC agree with this prediction when we use the same mechanisms as those in the continuum model. We used the simulations to examine other effects not in the continuum model that might increase the ripple growth rate: multiple defects per ion and Ehrlich-Schwoebel (ES) barriers to prevent the recombination of vacancy and adatom defects The multiple traces on figure 2 correspond to the results of these studies. Although they have a small effect on increasing the ripple growth rate, they cannot account for the large factor difference between the experiments and model.

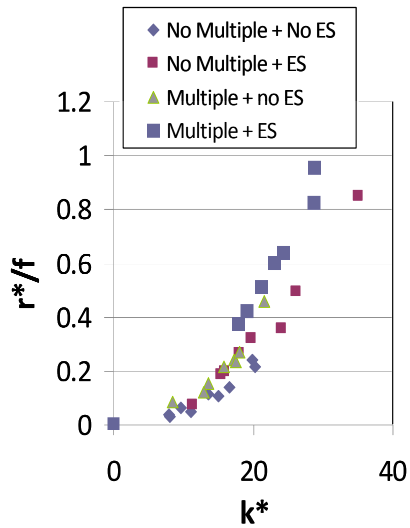

Figure 10. KMC results of effects of multiple defects and ES barrier on ripple growth

<u>Ion-induced stress as ripple driving force</u>

Stress induced by ion bombardment is another possible mechanism for enhancing ripple formation. This was incorporated into a theory that combines effects of curvature-dependent sputtering yield (as in the standard Bradley-Harper (BH) theory of ripple formation) with the effect of stress to form patterns (known as the ATGS theory). As shown in figure 11, stress in the layer is predicted to strongly modify the ripple growth rate (r*). At low stress, *r** is given by the BH results from the Bradley-Harper instability theory (green line in figure), but as the stress increases, the ripple formation becomes more like the stress-induced ATGS instability (blue line in figure).

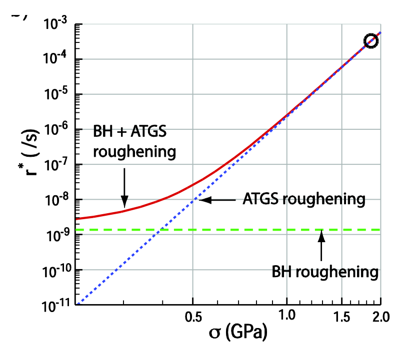

Figure 11. Results of model for effect of stress on ripple growth rate.

<u>Measurements of ion-induced stress</u>

We used wafer curvature to measure the stress induced by the ion bombardment of Si surfaces. Careful measurements are needed because the stresses are small and there

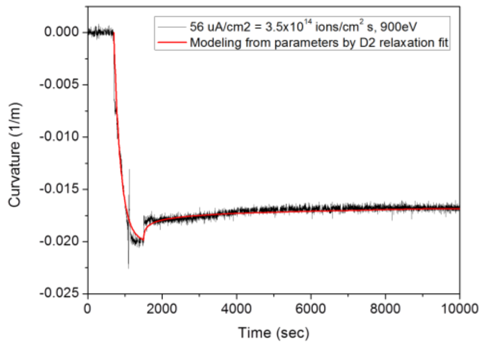

Figure 12. Stress vs time during sputtering. Solid line is fit to bimolecular annihilation model.

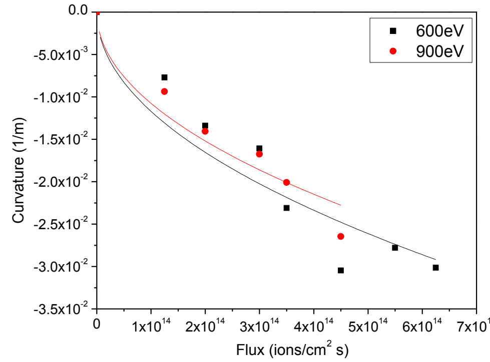

Figure 13. Measurement of ion-induced stress in Si vs ion flux with fit to our model of ion-induced relaxation.

are many potential artifacts such as thermally induced stress. Measurements of the stress as a function of time are shown in figure 12. The stress becomes increasingly compressive and then saturates at a steady-state value that depends on the flux. This is the first time that the flux dependence of ion-induced stress has been seen which shows that the stress is mediated by the kinetics of the ion-induced defects. The flux dependence of the steady-state stress is shown in figure 13. We also find that the stress relaxes partially when the ion beam is terminated (also shown in figure 12).

Model for ion-induced stress in amorphous Si

We developed a kinetic model to explain our measurements of stress induced by low energy ion sputtering of Si surfaces. This model is based on understanding how the steady state is determined by a balance between stress generated by ion implantation and relaxation processes in the amorphized Si. The relaxation occurs by viscous flow, but the viscosity is enhanced by the non-equilibrium concentration of defects when the ion beam is on. The evolution of the measured curvature (K) is governed by the following equation:

$$\frac{dK}{dt} = fK_0 - \frac{1}{\eta}K - fyK \qquad (4)$$

where f is the flux and y is the sputter yield. The fluidity ($1/\eta$) is taken to be proportional to the concentration of flow defects based on previous work by Witvrouw and Spaepen:

$$\frac{1}{\eta} = \alpha C \qquad (5)$$

where C is the non-equilibrium concentration of defects induced by the ion beam. The defect concentration is described by a balance between creation and annihilation mechanisms:

$$\frac{dC}{dt} = fC_0 - D_1C - D_2C^2 - fyC \tag{6}$$

where D_1 and D_2 are coefficients for either unimolecular or bimolecular processes. Fitting our results to this model indicates that the bimolecular annihilation mechanism gives the best agreement with the measurements of stress vs flux (solid line in figure 13) and the time evolution of the stress (figure 12). These results are a critical extension of earlier studies of viscous relaxation that connect ion-induced relaxation with other relaxation processes in amorphous Si.

<u>Surface morphology of alloys – thermodynamics, segregation and strain</u>

Alloy structures such as core-shell particles, heteroepitaxial multilayer's, nanowires and surface ripples have received a lot of attention in recent years due to their applications in logic, energy storage and optoelectronics. In typical growth conditions, the surfaces of these structures are usually faceted i.e. they adopt low-energy singular crystalline orientations. For alloy systems, the growth law for a fully faceted structure requires the specification of the normal velocity of each facet, the incorporation rate of each alloy component on the surface, and the exchange of surface atoms with the bulk. The latter process requires consideration of both surface segregation and possibly bulk material transport. By using only fundamental concepts of thermodynamics, recently, we derived the governing equations for the growth of strained and fully faceted two-component crystals in regimes where surface material transport may be governed by surface attachment limited kinetics or surface diffusion limited kinetics.

<u>Molecular dynamics simulations of ion-induced stress</u>

Molecular dynamics simulations have been developed to study the stress evolution in fcc metals (with Prof K.S. Kim's group). We have discovered a new mechanism to explain the "sawtooth" behavior in some metals (Ni, Cu, Ag in figure 14). In these systems, we find that the interstitial point defects aggregate into platelets below the surface surrounded by a dislocation loop. These loops are highly mobile and collect more point defects as they sweep below the surface. When the platelets become

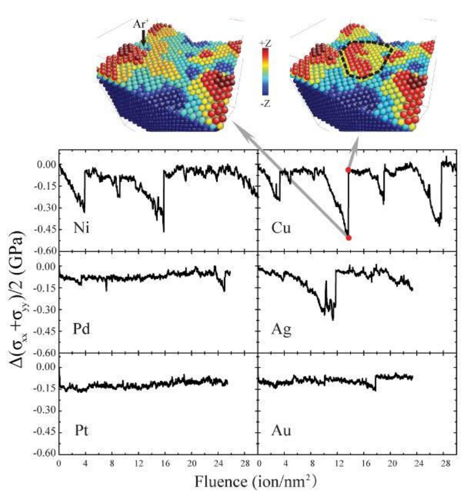

Figure 14. MD calculations of stress evolution during Ar bombardment on six f.c.c. metals with incident energy of 0.5 keV. (Top) Atomic plateau formation induced by the abrupt release of compressive stress.

sufficiently large, they cause the dislocation to cross-slip and glide to the surface. This causes the formation of an atomic plateau on the surface (shown by the images at the top of the figure) and relieves the stress in the layer (as indicated by the arrows on the stress plot). This mechanism couples the stress and morphology evolution in a different way than the Asaro-Tiller–Grinfeld instability and we are working to understand how it affects pattern formation on the surface.

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1. W. L Chan and E. Chason, "Making Waves: Kinetic Processes Controlling Surface Evolution during Low Energy Ion Sputtering", Applied Physics Reviews, J. Appl. Phys. 101, 121301 (2007).

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3. "Stress-enhanced Pattern Formation on Surfaces during Low-Energy Ion-Bombardment", N.V. Medhekar, W. L. Chan, V.B. Shenoy, E. Chason, J. Physics Cond Mat. 21, 224021 (2009).

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Graduate student progress: The program has supported the effort from several graduate students and the partial effort of one post-doc:
Wai Lun Chan (Asst. Prof. U of Kansas): measured the evolution of ion-induced ripples under different kinetic conditions.
Yohei Ishii (Hitachi): performed experiments to measure stress and composition modulations during sputtering.
Nikhil Medhekar (Monash U.): performed analysis of stress effects on ripples.
Rassin Grantab: performed MD simulations of ion-induced stress.
M.S. Bharathi (post-doc, Institute of High Performance Computing, Singapore): worked on KMC simulations of ion-induced pattern formation.

COMPREHENSIVE LIST OF PUBLICATIONS AND PRESENTATIONS FROM THIS DOE PROGRAM

The following list contains the publications and presentation made under this DOE program (9/01 – 11/30/2012; some appeared after program was ended).

PUBLICATIONS

1. “Observation of ion-induced ripples in Cu(001)”**,** Wai Lun Chan, Niravun Pavenayotin, Eric Chason, MRS Symp. Proc vol. 777, (2003)

2. “Spontaneous formation of patterns on sputtered surfaces”, Eric Chason, M. Aziz, Scripta Mat. 49, 953 (2003)

3. “Kinetics of ion-induced ripple formation on Cu(001) surfaces**,”** Wai Lun Chan, Niravun Pavenayotin, Eric Chason, Phys. Rev. B69, 254413 (2004)

4. “Influence of step-edge barriers on the morphological relaxation of nanoscale ripples on crystal surfaces,” V. B. Shenoy, A. Ramasubramaniam, H. Ramanarayan, D. T. Tambe, W-L. Chan, and E. Chason, Phys. Rev. Lett. 92, 256101 (2004)

5. “Relaxation kinetics of nano-ripples on cu(001) surface,” W. L. Chan, A. Ramasubramaniam, V.B. Shenoy, E. Chason, Phys. Rev. B 70, 245403 (2004)

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7. “Transient topographies of ion patterned Si(111),” Ari-David Brown, Wai Lun Chan, Eric Chason, Jonah Erlebacher, Phys. Rev. Lett. 95, 056101 (2005).

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10. “Kinetic mechanisms in ion-induced ripple formation on Cu(001) surfaces,” E. Chason, W.L. Chan, Nucl. Instr. Meth. B 242, 232 (2006).

11. “Morphology of ion sputtered Cu(001) surface: transition from unidirectional roughening to bidirectional roughening,” Wai Lun Chan, Eric Chason, Nucl. Instr. Meth. B242 228 (2006).

12. “Kinetic Monte Carlo simulations of ion-induced ripple formation: dependence on flux, temperature, and defect concentration in the linear regime,” E. Chason, W.L. Chan, M.S. Bharathi, Phys. Rev. B 74, 224103 (2006)

13. “Low energy ion bombardment and surface topography: continuum theories and kinetic monte carlo simulations,” in Ion Beam Science: Solved and Unsolved Problems, Eric Chason and Wai Lun Chan, Mat. Fys. Medd. Dan. Vid. Selsk, pp. 207 (2007)

14. “Kinetic phase diagram for morphological evolution on cu(001) surfaces during ion bombardment,” Eric Chason and Wai Lun Chan, Nucl. Instr. Meth. B 256, 305 (2007).

15. “Surface stress induced in cu foils during and after low energy ion bombardment,” Wai Lun Chan, Eric Chason, C. Iamsumang, Nucl. Instr. Meth B257, 428 (2007)

16. “Making waves: kinetic processes controlling surface evolution during low energy ion sputtering,” Wai Lun Chan and Eric Chason, Applied Physics Reviews, J. Appl. Phys. 101, 121301 (2007).

17. “Orientation of nano-grains in hard-disk media on ion-beam textured substrates,” Y. Maekawa, K. Sato, E. Chason and T. Mizoguchi, IEEE Trans. Magn. 43, 2169 (2007).

18. “Compositionally modulated ripples induced by sputtering of alloy surfaces,” V. B. Shenoy, W. L. Chan, and E. Chason, Phys. Rev. Lett. 98 (2007)

19. "Spontaneous patterning of surfaces by low energy ion beams," in Materials Science with Ion Beams, E. Chason and W.L. Chan, ed. H. Bernas (Springer Verlag, Berlin, 2010).

20. "Irradiation stress in Cu induced by low energy ions: experiment and modeling," Wai Lun Chan , Eric Chason, J. Vac. Sci. Tech. A26, 44 (2008)

21. "DOE panel report on basic research needs for materials under extreme environments," E. Chason (one of multiple authors), DOE workshop on Materials Under Extreme Environments (2008).

22. "Dynamics of nanoscale ripple relaxation on alloy surfaces," A. Ramasubramanian and V. Shenoy, Phys,. Rev. E 77, 1 (2008).

23. "Kinetic composition locking on faceted alloy surfaces", V.B. Shenoy, A. Ramasubramanian, Acta Mat 57, 196 (2009)

24. "Kinetic Monte Carlo simulations compared with continuum models and experimental properties of pattern formation during ion beam sputtering", E. Chason, W. L. Chan, J. Physics Cond Mat. 21, 224016 (2009).

25. "Stress-enhanced Pattern Formation on Surfaces during Low-Energy Ion-Bombardment", N.V. Medhekar, W. L. Chan, V.B. Shenoy, E. Chason, J. Physics Cond Mat. 21, 224021 (2009).

26. "Stress control in polycrystalline thin films-reduction in adatoms diffusion into grain boundaries via surfactants", Yi Yang and Hanchen Huang S. K. Xiang, Eric Chason, Appl Phys Lett. 96, 211903 (2010)

27. "Evolution of morphology and composition in three-dimensional fully faceted strained alloy crystals", Vivek B. Shenoy, Journal of the Mechanics and Physics of Solids 59 (2011) 1121–1130

28. "Surface nanopatterning mechanisms by keV ions: linear instability models and beyond", E. Chason, V. Shenoy, Nucl. Instr. Meth. B272, 178 (2012).

29. "Kinetic Monte Carlo simulation of ripple formation by sputtering: effects of multiple defects and Ehrlich-Schwoebel barriers", Y. Ishii, W.L. Chan, E. Chason, Nucl. Instr. Meth. B272, 188 (2012).

30. "Nanoscale mechanisms of surface stress & morphology evolution in FCC metals under noble-gas ion bombardments", Sang-pil Kim, Huck Beng Chew , Eric Chason, Vivek Shenoy and Kyung-Suk Kim, Proc Royal Society A 468, 2550 (2012).

31. “Simulation studies of low energy ion induced pattern formation”, W. L. Chan and E. Chason, in Ion Beam Induced Surface Nanostructuring of Materials, edited by T. Som (Pan Stanford, Singapore)

32. “Stress evolution in Si (001) during low energy ion bombardment”, Yohei Ishii1, Charbel S. Madi, Michael J. Aziz and Eric Chason, J. Materials Res. (acccepted, 2014 in press)

PRESENTATIONS

Invited Conference

1. “Ion-induced ripple formation in Cu(001) *(invited*),” Eric Chason, Wai Lun Chan, Ion Beam Modification of Materials (IBMM) 2004, Monterey CA, 9/5-10/2004

2. “Kinetic Monte Carlo simulations of ion induced patterning,” *(invited*), Eric Chason and Wai Lun Chan, WE-Heraeus-Seminar: Ions at Surfaces: Patterns and Processes, Bad Honnef, Germany, June 19-23, 2005.

3. “Ion-induced pattern formation: continuum theories, experiments and Kinetic Monte Carlo simulation” *(invited*), Eric Chason, Ion06: Ion Beam Science: Unsolved and Solved Problems, Copenhagen, Denmark, 5/1-5/2006

4. “Understanding ion-induced pattern formation: effects of kinetic parameters” *(invited*), E. Chason and W.L. Chan, International Conf. On Atomic Collisions in Solids (ICACS), Berlin, Germany, 7/21-26/2006.

5. “Kinetic mechanisms controlling ion-induced pattern formation” *(invited*), Eric Chason and Wai Lun Chan, MRS Fall meeting, Boston, MA 11/27-12/1/2006

6. “Ion beam patterning in the linear instability regime: kinetic mechanisms, persistent puzzles and new capabilities” *(invited*), E. Chason, W.L. Chan, N. Medhekar, V. Shenoy, Nanopatterning via Ions, Photon beam and Epitaxy, Sestri Levante, IT, 9/23-27/2007.

7. “Ion patterning: persistent puzzles and new directions” *(invited*), E, Chason, W.L. Chan, N. Medhekar, V. Shenoy, MRS Fall 2007, Boston, MA

8. “Simulations and experiments of ion beam patterning in the linear instability regime” (*invited*), Eric Chason, Wai Lun Chan and Vivek Shenoy, Workshop on self-organized nanostructures by low-energy ion beam erosion, Dresden, October, 2008

9. Invited talk, V. Shenoy , Nanoelectronic devices for defense and security conference, Ft. Lauderdale, FL, October 1, 2009.

10. Invited talk,,V. Shenoy, National Renewable Energy Laboratory workshop on energy-relevant thin films and nanostructures, Denver, CO, October 18, 2009.

11. Invited talk,V. Shenoy, MRS Fall Meeting, Boston, Dec. 2009

12. Invited talk, V.B. Shenoy, SIAM Conference on Mathematical Aspects of Materials Science, May 24, 2010.

13. Invited talk,,V. Shenoy, SIAM meeting on Mathematics of Materials Science, Philadelphia, May 25, 2010.

14. Invited lecture, V.B. Shenoy, Institute of Materials, Microelectronics and Nanosciences of Provence, Marseilles, France, June 15, 2010.

15. Invited lecture, V.B. Shenoy, Centre de Recherche sur l'Htro-Epitaxie et ses Applications, Nice Sophia-Antipolis, France, June 24, 2010

16. "Surface nanopatterning mechanisms by keV ions: linear instability models and beyond" *(invited*), E. Chason, V. Shenoy, IBMM (Ion Beam Modification of Materials) 2010 Montreal Aug. 2010

17. "Ion-induced relaxation in amorphous silicon: effects on stress and ripple morphology" *(invited*), E. Chason1 and Y. Ishii, Workshop on Nanoscale Patterning, Madrid, Sept. 2011

18. "Surface pattering mechanisms by keV ions: Coupling among energetic ions, surface kinetics, stress and composition" *(invited*), Eric Chason and V. Shenoy, COSIRES (Computer Simulations Of Radiation Effects in Solids), June 24-29, 2012, Santa Fe, NM

Invited University/Industry

1. "Kinetic mechanisms in ion-induced ripple formation: measurements and KMC simulations" *(invited*), E. Chason, Genova University, Genova, Italy, April 226, 2005

2. "Spontaneous pattern formation on sputtered surfaces "*(invited*), Eric Chason, GE Global Res. Center, Niskayuna, NY, 6/4-5/2006.

3. "Pattern formation on sputtered surfaces: experiments and kmc simulations" *(invited*), Eric Chason, Lawrence Livermore National Labs, Livermore, CA, 7/11/2006.

4. "Influence of non-equilibrium conditions on thin film stress and surface morphology evolution" (*invited*), Eric Chason, Washington University, St Louis, MO, 3/25/2007.

5. “Effects of high flux/low energy ions” (*invited*), E. Chason, DOE Workshop on Basic Research Needs for Materials under Extreme Environments, Bethesda, MD, 6/10-14/2007

6. “Influence of non-equilibrium conditions on thin film stress and surface morphology evolution” (*invited*), Eric Chason, Boston University, Feb. 2008

7. “Recent work in developing, characterizing and understanding advanced thin film materials”, E. Chason, Rogers Corp, Dayville, CT, 1/29/2009

8. Applied Mathematics Focused Research Kickoff meeting, V. Shenoy, University of Michigan, November 14, 2009.

9. V. Shenoy, Mechanical Engineering Colloquium, University of Houston, Houston, TX, November 12, 2009.

10. V. Shenoy, Materials Science Colloquium, University of Illinois, Urbana Champaign, December 7, 2009.

11. Distinguished Theory Lecture, V.B. Shenoy, Chemical and Materials Sciences Division, Oak Ridge National Laboratory, October 15, 2010.

Contributed presentations

1. “Observation of ion-induced ripples in Cu(001)”, W. L. Chan, N. Pavenayotin, E. Chason, MRS Spring 2003

2. “Temperature Dependence of Sputter Ripples on Cu(001) Surfaces,” W.L. Chan and E. Chason, MRS Fall 2003

3. “Morphology of ion sputtered Cu(001) surface: transition from unidirectional roughening to bidirectional roughening,” Wai Lun Chan, Eric Chason IBMM, Monterey, CA, 9/2004

4. “Temperature and flux dependence of ion induced ripple: a way to study defect and relaxation kinetics during ion bombardment,” W. L. Chan and E. Chason, MRS Fall 2004

5. “Morphological phase diagram of sputtered Cu(001) surface: measurement of the interplay between roughening and relaxation,” W. L. Chan and E. Chason, WE-Heraeus-Seminar, Ions at Surfaces: Patterns and Processes Bad Honnef, Germany, 6/19-23/2005

6. “Measurement of stress in thin Cu foil during low energy ion bombardment,” Wai Lun Chan, Eric Chason, C. Iamsumang, Ion Beam Modification of Materials (IBMM) 2006, Taormina, IT, 9/18-22/2006.

7. “Orientation of nano-grains in hard-disk media on ion-beam textured substrates,” Y. Maekawa, K. Sato, E. Chason and T. Mizoguchi, 10th MMM/Intermag Conf., Baltimore, MD, 1/7-10/2007.

14. “Stress due to low energy Ar ion bombardment: relation to ripple formation”, Y. Ishii, V. Shenoy, E. Chason, MRS Fall Meeting, Boston, Dec. 2009

15. “Kinetic Monte Carlo simulation of ripple formation by sputtering: effects of multiple defects and Ehrlich-Schwoebel barriers”, Y. Ishii, E. Chason, IBMM 2010 Montreal Aug. 2010

16. “Stress evolution in Si (001) during low energy ion bombardment: defect creation/annihilation processes and viscous relaxation”, Yohei Ishii and E. Chason, Gordon research Conf. On Thin Films, Biddeford ME, July 2011