This is an open book, open notes exam.

There are four questions. To receive full credit, you must show your work.

The exam is designed to be taken in 1 hour 15 minutes.

Be sure to fill in your name and Purdue student ID at the top of the page.

DO NOT open the exam until told to do so, and stop working immediately when time is called.

100 points possible

1) 20 points
2) 20 points
3) 40 points
4) 20 points

I understand that if I am caught cheating in this course, I will earn an F for the course and be reported to the Dean of Students.

Read and understood: ____________________________

signature
1. Answer T/F for the following questions  (20 points)

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| T | F | 8 | BTI can occur in both NMOS and PMOS, but NBTI occurs only in PMOS.  
Note. I did mention that NBTI could occur in NMOS in accumulation as well, but this is not a typical mode of operation. |
| T | F | 9 | Field-induced polarization of Si-H bonds (and reduction in barrier energy) explains NBTI field acceleration. |
| T | F | 10 | The time exponent of NBFI is independent of temperature and field.  
Note. Dispersive diffusion could add slight temperature dependence to the exponent. |
| T | F | 11 | The logarithmic time dependence of trapping in thick oxides is also reflected in the 1/f noise of the corresponding system. |
| T | F | 12 | One must first decompose the degradation components (e.g. trapping vs. defect generation) before we uses the reaction-diffusion model to interpret the data. |
Problem 2: Structure of crystalline materials (10+10)

In this problem, we will use the Euler’s relationship to demonstrate that the impossibility of forming an infinite 2D periodic lattice with five sided ring \((N_p = 5)\) based only on atoms of coordination \(r\).

a) Explain why the relationship between \(V, E,\) and \(N\) for a periodic solid with 5-sided ring \((N_p = 5)\) should be written as \(2E = rV = 5N\). Here \(r\) is the coordination of the atom.

Each edge is shared by two neighboring atoms. For every atom \(V = 1\) with coordination number \(r\), there should be \(\frac{r}{2}\) edges, so:

\[
E = \frac{r}{2}V \quad \rightarrow \quad 2E = rV
\]

Each edge is also shared by two neighboring rings. If we isolate all the rings, then the total number of edges is \(N_pN\), which equals \(2E\). Therefore, for every 5-sided ring, correspondingly there should be \(\frac{5}{2}\) edges, so:

\[
E = \frac{5}{2}N \quad \rightarrow \quad 2E = 5N
\]

In summary:

\[
2E = rV = 5N
\]

b) Use the Euler’s relationship \(V - E + N \sim 0\), to determine coordination \(r\) of the ‘atom’. Is this \(r\) possible?

From the result derived in a), we can rewrite \(E\) and \(V\) in terms of \(N\): \(E = \frac{5}{2}N, V = \frac{5}{r}N\)

Plug in Euler’s relationship:

\[
\frac{5}{r}N - \frac{5}{2}N + N \sim 0
\]

\[
\rightarrow r = \frac{10}{3}
\]

This result contradicts to the fact that the coordination number is an integral. So 5-sided ring is impossible.
Problem 3: Coordination and Ring-sizes of an amorphous solid (10+10+10+10)

Recently, one of your classmates sent me a PNAS paper by S Zhang et al, Proc. Natl. Acad. Sci. USA, 2015, DOI: 10.1073/pnas.1416591112. The paper uses the first principle method to predict the existence of penta-graphene with 5-ring structures, see below. We will justify the results by Euler relationship.

In Lecture 5, we have seen that atoms of only one variety (e.g. coordination \( r = 3 \)) leads to ringsizes narrowly distributed around an average, \( \langle N_p \rangle = 6 \). This derivation explained why very large rings are improbable. The PNAS paper demonstrates the inverse: A unique ring-size \( (N_p = 5) \) can be realized if multiple types of atoms with different coordination \( (r = 3, r = 4) \) are allowed. We will use the Euler relationship to determine the fraction of 3-coordinated atoms (\( \alpha \)) and remaining fraction with 4-coordinated atoms \( (1 - \alpha) \) necessary to form the lattice with a unique ring-size.

a) Explain why the relationship \( 2E = (3\alpha + 4(1-\alpha))V = 5N \) describes a penta-graphene.

Each edge is shared by two neighboring atoms. For every atom \( V = 1 \) with coordination number \( r \), there should be \( \frac{1}{2} \times [3\alpha + 4(1-\alpha)] \) edges, so:

\[
E = \frac{[3\alpha + 4(1-\alpha)]}{2}V \quad \rightarrow \quad 2E = [3\alpha + 4(1-\alpha)]V
\]

Each edge is also shared by two neighboring rings. For every 5-sided ring, correspondingly there should be \( \frac{5}{2} \) edges, so:

\[
E = \frac{5}{2}N \quad \rightarrow \quad 2E = 5N
\]

In summary:

\[
2E = [3\alpha + 4(1-\alpha)]V = 5N
\]
b) Find \( \alpha \) by solving the Euler relationship, \( V - E + N \sim 0 \). Count the number of 3 and 4 coordinated atoms in the figure above. Does the ratio satisfy the value calculated?

From the result derived in a), we can rewrite \( E \) and \( V \) in terms of \( N \):

\[
E = \frac{5}{2} N, \quad V = \left[ \frac{5}{3 \alpha + 4(1 - \alpha)} \right] N
\]

Plug in Euler’s relationship:

\[
\frac{5}{3 \alpha + 4(1 - \alpha)} V N - \frac{5}{2} N + N \sim 0
\]

\[
\rightarrow \alpha = \frac{2}{3}, \quad (1 - \alpha) = \frac{1}{3}
\]

In the figure, there are roughly 15 atoms with \( r=4 \) and 33 atoms with \( r=3 \). This ratio is approximately satisfying the calculated \( \alpha \) value. Note that you cannot take a unit cell to estimate the ratio; in an amorphous material, the estimate is better as you increase the area of sampling.

c) Let us calculate the stability of penta-graphene using the Maxwell’s relationship.

Calculate the bond constraints by requiring that \( N_{r=3} = \frac{2}{3} N \) and \( N_{r=4} = \frac{1}{3} N \).

\[
N_{c}^{\text{bond}} = \sum_{r=1,k} n_r \left( \frac{r}{2} \right).
\]

\[
N_{c}^{\text{bond}} = \frac{2}{3} N \times \frac{3}{2} + \frac{1}{3} N \times \frac{4}{2}
\]

\[
= \frac{5}{3} N
\]

Next calculate the angle constraint by using the formula

\[
N_{c}^{\text{angle}} = \sum_{r=1,k} n_r \left( D - 1 \right) \left( 2r - D \right) / 2.
\]
\[ N_{c}^{\text{angle}} = \frac{2}{3} N \times (2 - 1) \times \frac{1}{2} (2 \times 3 - 2) + \frac{1}{3} N \times (2 - 1) \times \frac{1}{2} (2 \times 4 - 2) \]
\[ = \frac{7}{3} N \]

d) Using Maxwell’s formula, calculate \( M_{0} = D - N_{c}^{\text{bond}} - N_{c}^{\text{angle}} \). Explain why penta-graphene is likely to be more defective than graphene.

For penta-graphene:
\[
\frac{M_{0, \text{penta}}}{N} = D - \frac{N_{c}^{\text{bond}}}{N} - \frac{N_{c}^{\text{angle}}}{N}
\]
\[ = 2 - \frac{5}{3} - \frac{7}{3} \]
\[ = -2 \]

For graphene:
\[
\frac{M_{0, \text{graphene}}}{N} = D - \frac{N_{c}^{\text{bond}}}{N} - \frac{N_{c}^{\text{angle}}}{N}
\]
\[ = 2 - \frac{3}{2} - \frac{4}{2} \]
\[ = -\frac{3}{2} \]

\[ \therefore \frac{M_{0, \text{penta}}}{N} < \frac{M_{0, \text{graphene}}}{N} < 0 \]

So penta-graphene is a more stressful structure than graphene, which means it’s likely to be more defective.
4. NBTI problems (10+10)

(a) Based on the equations \( N_{IT} \times N_H(0) \sim k_F N_0 / k_R \) and \( N_{IT} = \int_0^\infty N_H(x) \, dx \), determine the time exponent associated with drift of \( H^+ \) species. Note that protons drift a distance \( x_{max} = \mu E t \) during stress time \( t \). Here, \( E \) is the electric field.

\[
N_{IT} \times N_H(0) \sim \frac{k_F N_0}{k_R} \quad \rightarrow \quad N_H(0) \sim \frac{k_F N_0}{k_R N_{IT}}
\]

For drift \( H^+ \), we have:

\[
N_{IT} = \int_0^{\mu E t} N_{H^+}(x) \, dx \\
= \int_0^\infty N_{H^+}(x) \, dx \\
= N_{H^+}(0) \times \mu E t \\
= \frac{k_F N_0}{k_R N_{IT}} \times \mu E t
\]

\[
\rightarrow N_{IT}^2 = \frac{k_F N_0}{k_R} x \mu E t \\
N_{IT} = \sqrt{\frac{\mu E k_F N_0}{k_R}} \frac{1}{t^{\frac{1}{2}}}
\]

The time exponent: \( n = \frac{1}{2} \)

(b) We have assumed that neutral H diffuses primarily into the oxide. One often wonders if the diffusion in the other direction, namely, into Si, would fundamentally change the time exponents. In this problem, you will convince yourself that this does not happen.

i) Draw the triangular H profile into the oxide, and s second triangular profile into silicon. Assume the distance travelled by H into oxide is \( \sqrt{2D_{ox} \, t} \), while that into silicon is \( \sqrt{2D_{si} \, t} \). The height of the triangle at the Si/SiO\(_2\) interface is \( N_H(0) \) for both triangles.
ii) Use the fact that $N_{IT}$ can be obtained by integrating the area under the curve of the triangular profile, to derive an expression for $N_{IT}(t)$. Did the exponent change by including diffusion into Si?

$$N_{IT} \times N_H(0) \sim \frac{k_F N_0}{k_R} \rightarrow N_H(0) \sim \frac{k_F N_0}{k_R N_{IT}}$$

For diffusive $N_H$, we have:

$$N_{IT} = \int_0^\infty N_H(x) \, dx$$

$$= \frac{1}{2} N_H(0) \times \left( \sqrt{2D_{Si} t} + \sqrt{2D_{SiO_2} t} \right)$$

$$= \frac{1}{2} \frac{k_F N_0}{k_R N_{IT}} \times \left( \sqrt{2D_{Si}} + \sqrt{2D_{SiO_2}} \right) \times t^{\frac{1}{4}}$$

$$\rightarrow N_{IT} = \frac{1}{2} \frac{k_F N_0}{k_R N_{IT}} \times \left( \sqrt{2D_{Si}} + \sqrt{2D_{SiO_2}} \right) \times t^{\frac{1}{4}}$$

We can see from the expression above, whatever there’s the $\sqrt{2D_{Si}}$ term or not, the time exponent $n$ is always equal to $\frac{1}{4}$, which means it doesn’t matter whether we include the effect of H diffusion into Si or not.