Simulating SiGe and Impurity Dependent Stress

1.0 Introduction

The simulation of stress during device fabrication is becoming increasingly important and is often now deliberately introduced during fabrication to enhance device performance. The induced stress can take the form of deposited amorphous materials, such as silicon nitride or can be induced epitaxially by the growth of silicon germanium (SiGe) for example.

Un-intensional stress is also added to or subtracted from the fabricated device simply as a result of necessary dopants. Boron and carbon being small atoms, add "contractive" stress to a structure whilst atoms larger than silicon, such as indium, induce stress that tries to create local expansion. Having said that, some larger atoms, such as arsenic, do not appear to add significant amounts of stress to the structure, and neither do atoms of a similar size to silicon such as phosphorus.

In a process simulator, the summation of all these local stresses has to be taken into account and then passed to the device simulator for analysis of the resulting strain on mobility, bangap, Nc and Nv etc.

2.0 Implementation

In ATHENA, germanium is treated as a dopant, so by default, the effects of germanium incorporation into the crystal lattice can be summed up locally with the stress resulting from all other dopants and stress inducing deposited films.

A viscous stress model has been incorporated into ATHENA with defaults for germanium, boron and carbon. The model is user definable for the XX and YY directions and takes the form of the following general quadratic equation:-

```
Stress = a(xx) + b(xx)N + c(xx)N2

Stress = a(yy) + b(yy)N + c(yy)N2
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where "N" is the impurity concentration. In general, the impurity induced stress will be approximately linear with concentration, so "a" and "c" will be relatively small normally. Germanium for example, has a slight "bowing" in the stress versus concentration curve which is taken care of by the quadratic form of the equation (the "c" coefficient). Currently, ATHENA has good defaults for germanium, carbon and boron. Others will be added as the information becomes available but the user can make any dopant create a stress dependency in the structure.

If the default values for germanium concentration stress dependency were to be input manually, the additional lines in the ATHENA input file would be as follows:-

```
impurity i.germanium silicon
Bxx.strain=-0.0366783
Cxx.strain=-0.000503222

impurity i.germanium silicon
Byy.strain=-0.0366783
Cyy.strain=-0.000503222
```

The formula can be applied to any impurity or any number of impurities by specifying the chemical dopant and the coefficients in an analagous way.

In the current implementation, all exposed surfaces are stress terminators (which is physically correct) and all other boundaries, typically the sides and bottom of the simulation domain, are reflective. In other words, if a dot of germanium dopant is simulated in a square of silicon, the resulting stress will be as if the sides and bottom of the simulation domain also have germanium dots that are located at a spot defined by mirror images of the sides and bottom. If the effect of reflective boundaries is not wanted, the user simply has to make the simulation domain larger, such that the unwanted stress no longer has an effect.

3.0 Usage

The impurity dependent stress model and the stress induced by differences in thermal expansion between different materials in the structure are solved self consistently. Consequently, it is always necessary to specify two temperatures to calculate the combined stress in the structure from these two different effects. If it is desired to isolate the effects of stress induced by the impurities alone, then simply specify the two temperatures as being equal, so no additional thermal expansion differences occur.

The impurity dependent stress calculations are invoked on the method statement.

When coupled with the stress statement, the syntax will be as follows:-

```
method dopant.stress

stress temp1=<celcius> temp2=<celcius>
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When creating a user defined impurity dependent stress model using the material statement syntax described in section 2, it is important to realize that the formula for

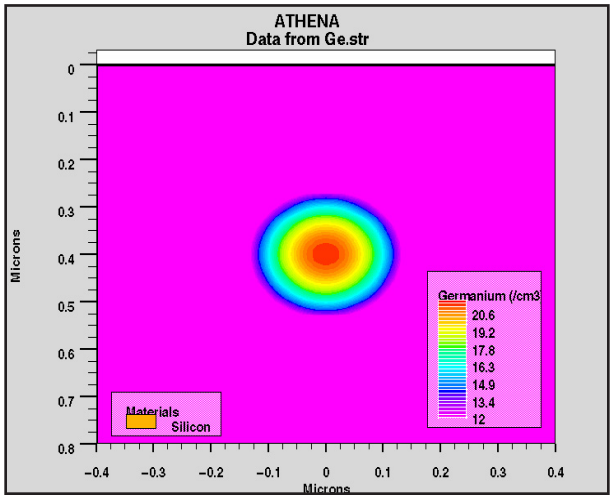

Figure 1. showing germanium impurity distribution for experiment 1 where the dopant is completely encapsulated within silicon.

impurity dependent stress that needs to be defined, is the formula which applies when no stress relief through strain relaxation has occurred. The user does NOT have to take into account the location of the impurity in the structure. Any stress relief that occurs in the structure as a result of the impurity's proximity to a free surface will be calculated automatically. In the following sections, two examples will be shown to help illustrate this point.

4.0 Test Example 1

In the first example, a "trivial" case is investigated, where no stress relief from strain can take place. The stress in the XX and YY directions should therefore be symmetrical and identical. A block of silicon, 0.8um x 0.8um, was defined with a "dot" of germanium doping in the middle. After an anneal, the "dot" was diffused to create a gradient of germanium concentration in the silicon. The resulting dopant distribution is shown in figure 1.

Since the germanium doping "dot" is completely encapsulated in silicon, almost no relief of stress can take place. The result will not be completely symmetrical, since the free silicon surface is not infinitely far away but the experiment is close enough to verify the correct implementation.

Figure 2 shows the resulting stress in the XX and YY directions respectively. As expected the stress in both XX and YY directions is symmetrical. Any slight differences are a result of the proximity free surface and the reflecting boundaries.

5.0 Test Example 2

This next example shows how the intrinsic stress defined using the syntax shown in section 2 is automatically modified by the viscous stress calculations that take into account the free silicon surface.

It is a physical requirement that the nett stress in a direction normal to a free surface must be zero. If it were not, the surface would simply lift off. The stress at the surface is relieved via the process of strain. It is this resulting strain which modifies the electrical properties of the semiconductor. Calculating the strain from a stress field in a well documented process and these transformation calculations are integrated into the device simulator. Further information on the mathematics of the strain transformation calculations from stress fields can be found in the ATLAS manual or other standard texts.

Figure 3 shows the new test structure used in this example. It is the same structure that was used in example 1 except that the top surface has been etched away to intersect with the SiGe "diffused dot", such that there is a non zero concentration of SiGe at the free surface.

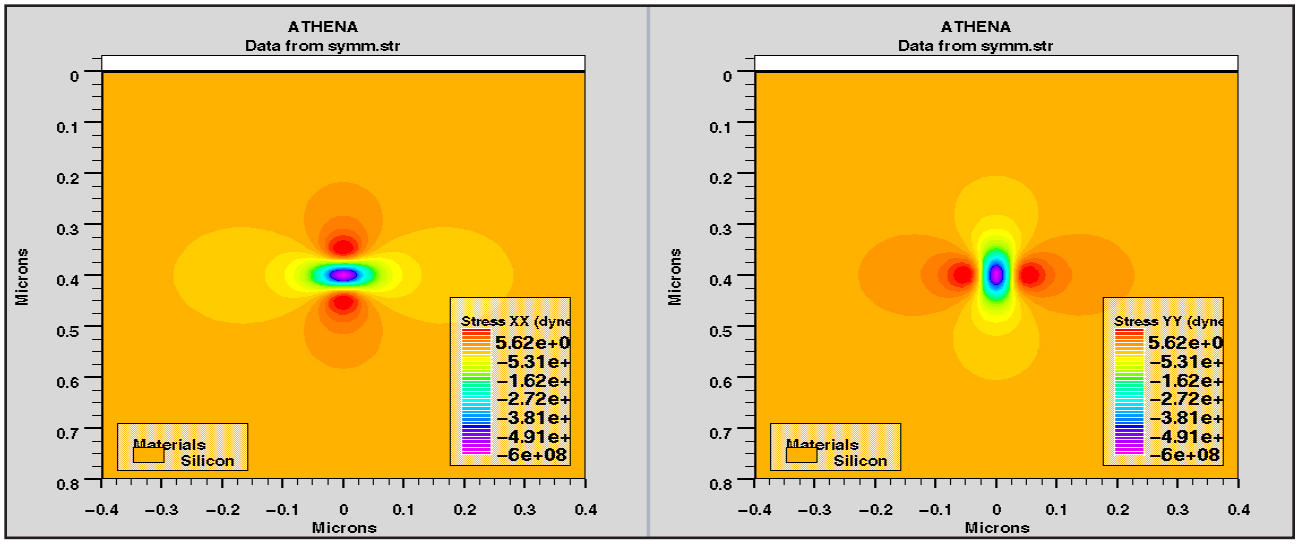

Figure 2. calculated stress fields in the XX and YY directions resulting from the buried SiGe dot shown in figure 1 .

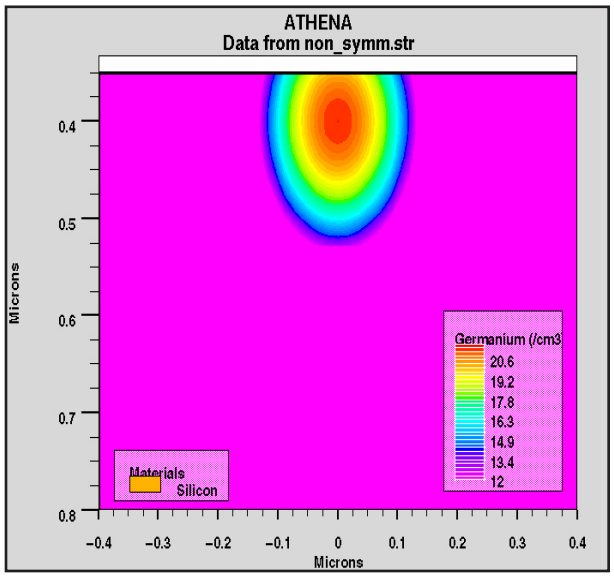

Figure 3 The test structure for experiment 2 showing the same SiGe "diffused dot" as in Figure 1, but with the surface of the structure etched away, leaving a non zero concentration of SiGe at the free surface.

The resulting stress fields are shown in figure 4. It will be immediately apparent that the stress fields in the XX and YY directions are no longer symmetrical as a result of the relief of the stress at the surface in the perpendicular YY direction. A cutline along the surface in the YY direction shows that the stress has been reduced to zero as expected, despite the presence of SiGe at the surface. The stress at the surface in the XX direction however, is non zero as a result of the SiGe at the surface.

6.0 Conclusions

A new impurity dependent viscous stress calculation has been implemented in ATHENA which is solved self consistently with additional stresses resulting from thermal differences of expansion. Since germanium in ATHENA is treated as a normal dopant, stresses for SiGe films are automatically included in the calculation of these stress fields. Stress resulting from all impurities and thermal expansion differences are solved and summed locally and self consistently throughout the device using a viscous formulation. Concentration dependent stress default values for germanium (and therefore SiGe), carbon (and therefore SiGeC) and boron impurities have been obtained from published references. The equations are user definable and modifiable for any impurity and take the form of an arbitrary quadratic to account for "bowing" in some of the stress versus impurity concentration curves.

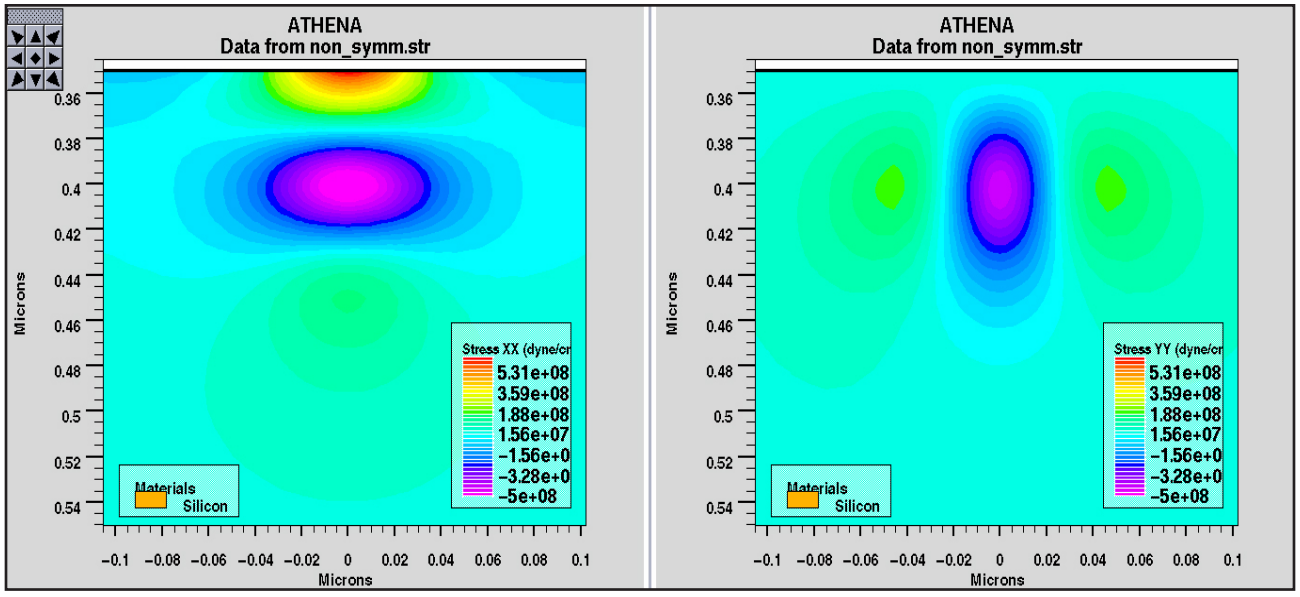

Figure 4 Resulting XX and YY direction stress fields as a result of the SiGe dot shown in Figure 3.