Electrically-Active Interfaces for Chemical Sensors

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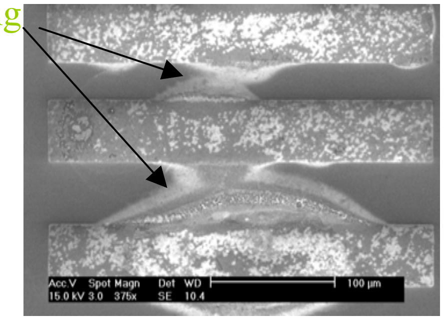
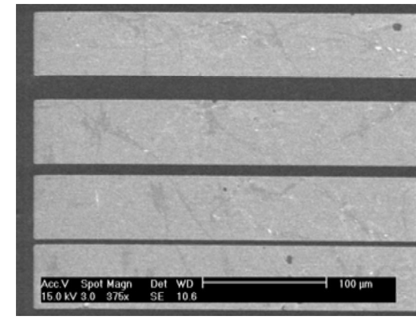
- The intrinsic properties of the semiconductor silicon carbide (SiC) allow it to be used in electronics at temperatures where silicon (Si) cannot be used. However, while the intrinsic properties of this wide bandgap semiconductor allow for higher operating temperatures, interfaces between dissimilar materials (e.g., metal-semiconductor) often interact at relatively low T. These interfaces (e.g., contacts) are necessary for solid-state gas sensors, which operate at high T.
- The images (upper and lower right) show homogeneous, single-phase PtSi contacts resulting from a controlled reaction between Pt and Si and which are predicted to be thermally stable with SiC (phase diagram, 1000 C).
- The traditional approach to forming ohmic contacts to p-type SiC is to anneal an Al-based contact (e.g., TiAl) on p+ SiC at temperatures ~1000°C. However Al-based contacts have morphological problems resulting from high processing or operating temperatures (upper left). These problems are associated with the high tendency for oxidation, phase separation with low melting point phases, a low eutectic temperature between Al and Si, and a non-uniform interface with the SiC substrate.
- Our results provide an understanding of the thermodynamics (how stable?) and the kinetics (how fast?) of metalSiC interfaces, which are critical for the reliability of high-temperature devices.
- For future work we plan to investigate conductive metal-oxides for thermodynamic, chemical, and electrical compatibility with both the semiconductor and the corrosive gas ambient at high T.

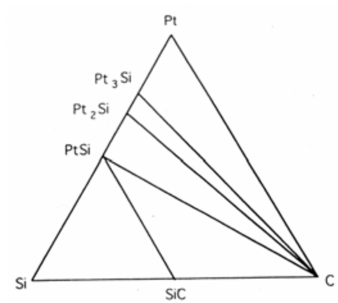
Conventional technology

shorting

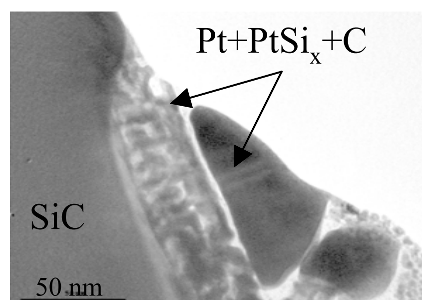


PtSi contacts developed at CMU

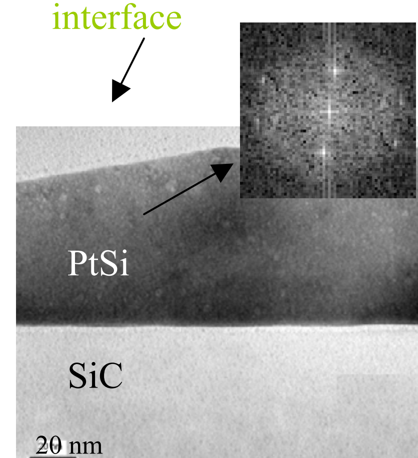




Uncontrolled reaction



Controlled reaction forms abrupt, stable interface



With new legislation and increasing attention on curbing the emission of pollutants into the atmosphere, chemical sensors that can be used to monitor and control these unwanted emissions are in great demand. However, many of the polluting processes and gases require sensors that can be operated at high temperatures (~300–800 °C).

The intrinsic properties of the semiconductor silicon carbide (SiC) allow it to be used in electronics at temperatures where silicon (Si) cannot be used. Therefore, there is strong interest in developing SiC-based devices for both military and civilian high-temperature electronics such as gas sensors that can be used at high temperatures and in aggressive environments. However, while the intrinsic properties of this wide band-gap semiconductor allow for the expansion of the current limits on operating temperature, interfaces between dissimilar materials (e.g., metal-semiconductor) often interact at relatively low temperatures. These interfaces (e.g., contacts) are necessary for all solid-state gas sensors.

In the example shown above, we compare the conventional contact technology (Al-Ti) for p-type SiC to single-phase PtSi contacts that we developed and studied at CMU. The traditional approach to forming ohmic contacts to p-type SiC is to anneal an Al-based contact (e.g., TiAl) on p+ SiC at temperatures around 1000°C. However, as shown in the SEM image (upper left) of a contact test pattern, Al-based contacts have morphological problems resulting from the high processing and/or operating temperatures. These problems are associated with the high tendency for oxidation, phase separation with low melting point phases, etc. In contrast, the PtSi contacts showed a smooth morphology (upper right) and no reaction with the SiC (TEM image with FFT 'diffraction' patter, lower right).

The fabrication process consists of sequential sputter deposition of the metal layers followed by annealing at ~1000 °C. The thicknesses of the Si and Pt layers resulted in a controlled reaction with the formation of the PtSi phase, which is predicted to be thermodynamically stable with SiC (middle left). The direct tie line between the PtSi phase and the SiC phase indicates that no new phases will form between them. On the other hand, one can notice that the Pt2Si and Pt3Si phases would not be in equilibrium with SiC. The phase diagram shown is for 1000 °C, which is the temperature required for the ohmic contact anneal. Our results show that under the right conditions the kinetics of the reaction between the Si and Pt layers is sufficiently fast to prevent an undesirable reaction with the SiC. If insufficient Si is present, the SiC reacts with the metal because of its low heat of reaction (lower left).

Our studies are resulting in an understanding of the reactions to yield single-phase contacts on SiC. We will be characterizing the PtSi contacts and conductive oxides as a function of temperature and gas exposure. We will characterize the reactions that occur in the presence of oxidizing gases.

Comparison of Ti/Al, Pt, and Pt/Si

Property	Al-Ti	Pt	PtSi
Average ρ_c (Ω-cm^2)	6.7×10^{-5}	2.3×10^{-4}	4.9×10^{-5}
Contact Morphology	Non-uniform	Non-uniform	Uniform
Standard Deviation of ρ_c	3.4×10^{-5}	3.83×10^{-5}	1.28×10^{-5}
Interface Roughness	Rough	Extremely rough	Flat and Abrupt
Reaction with SiC	Yes	Yes	No reaction
Residual Carbon	No	Yes	No
Thermal Stability	Unsuitable	Unsuitable	Suitable

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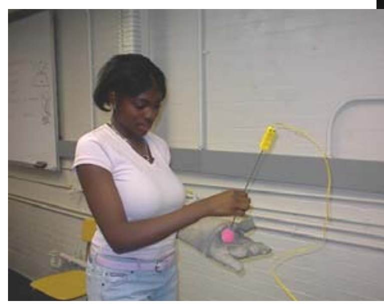
- The broader impacts can be divided into three new objectives: 1) to promote graduate student exchange via visits to and from Sweden, 2) to supervise an undergraduate research project pertaining to chemical sensors and 3) to introduce a lunch/speaker series designed to inspire and retain women graduate students and post-docs in materials science.
- The PI has continued her 5th year of involvement in the Engineering Your Future outreach program. The pictures show
  - *Middle school students measuring the low-temperature properties of silicone rubber and superconductors.*
  - *High school students oxidizing titanium and using it to make jewelry.*

Middle School Session



High School Session

1) To foster a strong collaboration with our European partner, annual meetings in both the U.S. and Europe are planned. In this way the graduate student can accompany his or her samples and help to perform the response measurements. Visits of approximately one month at a time will be encouraged. The PI has already visited Linköping University (August 2004) to discuss research and plan experiments.
2) We propose to supervise an undergraduate research project via a Research Experience for Undergraduates supplement request (to be submitted this fall). Our European partner has agreed to supply sensor structures for the undergraduate student to characterize via current-voltage measurements, SEM, etc.
3) The PI will be hosting a series of lunches designed to inspire women graduate students in materials science to continue along a profession in science and engineering. The idea is to hold approximately six lunches so that women graduate students and post-docs in materials science can come together as a group and share their ideas and similar experiences and to encourage them to consider various options for the future, such as a career in academia. To inspire discussion, for each lunch a speaker would be invited to give a short informal talk on a selected topic, such as how to balance personal and professional responsibilities and professional aspirations: academia vs. industry.
4) For the fifth year, the PI helped run the Engineering Your Future Workshop (sponsored by the Society of Women Engineers) for middle school and high school girls. The middle-school session comprised hands-on experiments of several classes of engineering materials, including semiconductors, superconductors, metals, ceramics, and polymers. Above is shown a student measuring the temperature-dependent properties of polymers and other students using the magnetic levitation effect to measure the transition temperature of superconductors. In the high school session (also shown above), the students oxidized titanium to make different types of jewelry.