**Socratic Prompting with Argo: Assessment**

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**Original Prompt:**

“Can you summarize how to reveal dislocations on SiC wafers to perform dislocation density analysis?”

**Socratic Reformulation:**

“What methods are used to reveal dislocations on SiC wafers, and how do these methods help in analyzing dislocation density?”

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| **Principles** | **(Follow-Up) Prompts** |
| **Dialectic** | **Original Prompt:**  “Can you summarize how to reveal dislocations on SiC wafers to perform dislocation density analysis?” |
| **Generalization** | **Follow-up Prompt 1:**  “What historical developments in dislocation analysis have influenced current techniques for SiC wafers? How can these insights help us generalize the approach to new materials or technologies?” |
| **Induction** | **Follow-up Prompt 2:**  “How does the process of revealing dislocations in SiC compare to similar processes in other semiconductor materials, such as silicon or gallium arsenide? What can we infer about the challenges specific to SiC from these comparisons?” |
| **Recollection** | **Follow-up Prompt 3:**  “What historical developments in dislocation analysis have influenced current techniques for SiC wafers? How can these insights help us generalize the approach to new materials or technologies?” |

1. **Motivation**

*Why is this problem important in chemistry/materials science?*

SiC is a wide bandgap semiconductor with high thermal conductivity and high breakdown electric field, which make it ideal to be used in high power and high temperature applications on power electronics. It has high hardness (9.0+) and resistant to oxidation and corrosion. Crystal defects, like grain boundary, and dislocations lead to failure of the system during operation. Thus, it is important to obtain single crystal wafers with low dislocation density is important. Even though industry can produce single crystal SiC crystals successfully, there is still need improvement on dislocations and how they analyzed. Since the material is chemically inert, the etching process requires high temperature chemical etching with usually KOH or NaOH. Developing alternative and safe solutions at low temperature is critical.

*What challenges exist in solving this problem using traditional LLM approaches?*

Traditional LLM try to guess chemical etchants by comparing with different materials without considering SiC is chemically inert. Thus, it suggests new solutions, which can be used only for surface cleaning process, without targeted etch pit reveal.

*How could a structured Socratic approach improve reasoning and outcomes?*

Socratic approach provided more specific response by summarizing methods to reveal dislocation density. It did not list step by step experimental procedure and also included alternative experiments, like X-ray topography, which was not suggested by traditional LLM.

1. **The Mixed Socratic Prompt Method Used**
2. **What Are the Prompts Used?**

***Original Prompt:***

“Can you summarize how to reveal dislocations on SiC wafers to perform dislocation density analysis?”

***Socratic Reformulation:***

“What methods are used to reveal dislocations on SiC wafers, and how do these methods help in analyzing dislocation density?”

1. **What Are the Outcomes of This Example?**

*How did the LLM refine its answers over iterations?*

Traditional LLM answered with step-by-step experimental procedure starting from cleaning, polishing, and to microscopic analysis. It was lack of focus. When mixed Socratic approach was used, reformulation improved the outcome and follow-up questions eased to keep the LLM in focus.

*What key insights or discoveries emerged?*

Socratic approach provided alternative analysis methods to chemical etching at high temperature, which are safer and non-destructive.

*Any unexpected results or challenges?*

Both traditional LLM and Socratic LLM suggests HF/HNO3 as a solution to be used for etch pit formation. However, traditional LLM answered the question “what about HF/HNO3 solution. Is it used for etch pit reveal?” with “oxide removal and surface smoothing”. This solution is not reported in the literature used for etch pit reveal process.

1. **Comparison to a Non-Socratic Approach**

*How did reasoning depth, self-correction, and hypothesis refinement compare?*

The traditional approach seems not to be following the conversation, rather answering questions outside of the context.

*Would a traditional direct-answer prompt have produced different results?*

Traditional approach led to more generalized response with step by step experiment design. Socratic approach, on the other hand, responded with a focused answer, even with alternatives to chemical etching.

*Did the Socratic method improve clarity, adaptability, or accuracy?*

Overall, Socratic method improved scientific prompting and accuracy. Answers are focused and short. Follow-up prompts helps the scientist to ask correct question without diverting the conversation.